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Mathematical Modelling of Migration of Volatile Compounds into Packaged Food via Package Free Space. Part I: Cylindrical Shaped Food

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ABSTRACT

During storage, some volatile constituents of packaging materials may migrate, through the air, into foodstuff. To predict migrants concentration in a cylindrical food at a given storage time, two-dimensional transient diffusion in a cylinder was solved by finite the difference method. A computer program was developed to model migrant concentration in cylindrical packaged food. The mathematical model was then validated by experimental tests applied to a high humidity food analog stored in wooden packaging. The food analog was made of 2% of agar and 98% of distilled water (w/w). Volatile compounds extracted from poplar trees were used as diffusing gas. The poplar tree is a major source of wood in food packaging in France. The gas concentrations in volatile compounds were detected by chromatography coupled with mass spectrometry. From these components, benzaldehyde was selected as the volatile component for experimental model validation. The benzaldehyde diffusion coefficient in simulated food was equal to $1{\cdot}1 \pm 0{\cdot}1 \times 10^{-6}\ cm^2\ s^{-1}$. Partition coefficients of benzaldehyde between packaging material and free space air of packaging and also between air and food analogs were determined.

NOMENCLATURE

ADI	Alternating direction implicit
α	Transfer coefficient at the boundary
C	Concentration ($\mu g\ g^{-1}$)

*To whom correspondence should be addressed.

C_R	Volatile concentration at cylinder radius extremity
C_o	Concentration at equilibrium
C_L	Volatile concentration at cylinder axial extremity
$[c^{*n'}_{i,j}]$	Concentrations at intermediate time which are found in first stage
$c^{*n}_{i,j}$	Dimensionless concentration at initial time which is known
$[c^{*n+1}_{i,j}]$	Dimensionless concentrations at time interval of duration ($t+\Delta t$ or second half time step)
C_w	Volatile concentration in wood package ($\mu g\, g^{-1}$)
C_X	Volatile concentration at the package surface ($\mu g\, g^{-1}$)
D	Volatile diffusivity in cylindrical food analog ($cm^2\, s^{-1}$)
d	Diameter (cm)
Δz^*	Increment of normalized length
Δr^*	Increment of normalized radius
GC	Gas chromatography
HSGC	Head space gas chromatography
i,j	Signify the nodes location
I,J	Space parameters
LL	Time counter parameter
MS	Mass spectrometry
Nu	Nusselt number
Pr	Prandtl number
r^*	Normalized cylinder radius
R	Cylinder radius (cm)
Ra	Raleigh number
Sh	Sherwood number
TDMA	Tridiagonal matrix algorithym
t	Time (seconds)
t^*	Dimensionless time
X	Thickness of the package
Z^*	Normalized cylinder axe.

INTRODUCTION

For food safety, one of the major problems is related to molecular diffusion from packaging material to food during storage. Mass transfer within food/packaging systems are well documented (Blumethanl, 1997). Several authors evaluated the diffusion of packaging film components to foods in the case of direct contact between food and packaging material (Chang *et al.*, 1988; Mercer *et al.*, 1991; Goydan *et al.*, 1990; Begly & Hollifield, 1990; Page *et al.*, 1992; Castle *et al.*, 1993; Desobry & Hardy, 1994; Jickells *et al.*, 1991; Kim-Kong, 1990; Naveh *et al.*, 1983; Nrishina, 1988; Tandon & Bhowmir, 1986). If there is no contact between food and packaging, only volatile molecules can migrate into food and the corresponding mass transfer is more complex. Volatile molecules evaporate at the packaging surface, cross the packaging/air interface, migrate through the air, cross the air/food interface and diffuse into the food. For instance, this kind of transfer occurs often for foods stored in wood boxes (fruits, vegetables, poultries, cheeses, etc.). Bankova *et al.* (1987) and Green Away *et al.* (1989) highlighted that wooden packaging materials produced from popular trees contains volatile compounds such as polyphenols, phenylaldehydes or ketones that can migrate into foods through the packaging head space. Migration depends expressly upon volatile compound concentration in the packaging material, its partitioning coefficient (packaging material/food) and time (Gilbert, 1976, 1979).

A mathematical model is a tool to predict the migration of volatile constituents from packaging materials to foods during storage. Mathematical modelling alone cannot replace measurements; to make measurements for every geometry and every set of materials is impossible. Mathematical models of migration are especially important in planning experiments and formulating legislation (Lum Wan *et al.*, 1995).

Differential equations governing mass transfer can be solved for simple boundary conditions and geometries (Crank, 1975), while numerical methods have to be used for the more complex conditions with the help of a computer (Croft & Lilley, 1977; Lomauro & Bakshi, 1985). Finite difference methods facilitate the solution of differential equations governing mass transfer (Hsu, 1981, 1983; Bakshi & Singh, 1980).

One-dimensional moisture transfer in packaged cereal–fruit systems by finite difference methods has been studied by Sapru and Labuza (1996). To solve two-dimensional diffusion in a cylindrical shape, it is necessary to use a performant method. In this paper, the alternative direction implicit (ADI) method for solution of the finite difference equation of transient problems which overcomes the time step restriction for stability and involves the solution of many equations, as explained by Croft and Lilley (1977), was applied.

The aim of this study was to develop a mathematical model to predict distribution of volatile concentration, at any time, in packaged cylindrical food via package free space and to validate this model experimentally.

MATERIALS AND METHODS

Theory

Model hypothesis

Migration was assumed to occur from the packaging material, through the package free space, into the cylindrical food. Packaging material and cylindrical food were considered homogeneous and isotropic. Isothermal transfer at 20°C was assumed. This paper does not take into account possible chemical or biological changes during food storage. The diffusion coefficient was considered to be constant and independent of concentration and diffusion direction. It was assumed that no migration loss outside of the package happened. Inside the package, concentration equilibrium with free space air was verified. Diffusion in the cylindrical food was considered to occur both in the radial and axial directions. Diffusion was studied in a quarter of the cylinder because of symmetric conditions.

Mathematical model

Mass conservation at the package surface as a plane sheet requires that:

$$\left(-D_{\mathrm{w}}\frac{\partial c}{\partial x}\right)_{x=X}=\alpha(c_{X}-c_{\mathrm{o}}). \tag{1}$$

No concentration gradient was assumed in the package material thickness ($\partial c/\partial x = 0$) because thickness ($X$) is negligible compared to the width and/or length of the package. So we have:

$$c_X = c_o.$$

On the other hand, there is a concentration equilibrium between inner surface of packaging material and internal head space.

The general solution of two-dimensional transient diffusion in an isotropic cylinder has been demonstrated by Crank (1975) as follows:

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{\partial^2 c}{\partial z^2} + \frac{1}{r}\frac{\partial c}{\partial r}\right). \tag{2}$$

The governing initial and boundary conditions to eqn (2), adapted to actual packaging conditions in this paper, are

$$t = 0, \quad c = 0, \quad \text{and for } t > 0:$$

$$r = 0, \quad \left(\frac{\partial c}{\partial r}\right)_{r=0} = 0 \quad \text{and} \quad r = R, \quad \left(-\frac{\partial c}{\partial r}\right)_{r=R} = \alpha(c_R - c_o),$$

$$z = 0, \quad \left(\frac{\partial c}{\partial z}\right)_{z=0} = 0, \quad \text{and} \quad z = L, \quad \left(-D\frac{\partial c}{\partial z}\right)_{z=L} = \alpha(c_z - c_o).$$

By introducing the following dimensionless parameters,

$$c^* = \frac{c - c_o}{-c_o}, r^* = \frac{r}{R}, z^* = \frac{z}{R}, t^* = \frac{tD}{R^2}, l^* = \frac{L}{R},$$

we obtained eqn (3) with new initial and boundary conditions

$$\frac{\partial c^*}{\partial t^*} = \frac{\partial^2 c^*}{\partial z^{*2}} + \frac{\partial^2 c^*}{\partial r^{*2}} + \frac{1}{r^*}\frac{\partial c^*}{\partial r}, \tag{3}$$

$$t^* = 0, \quad c = 0, \quad c^* = 1 \tag{4}$$

and for $t^* > 0$

$$\text{at} \quad r^* = 0, \quad \frac{\partial c^*}{\partial r^*} = 0, \tag{5}$$

$$\text{and at} \quad r^* = 1, \quad \left[\frac{\partial c^*}{\partial r^*} + \frac{\alpha R}{D} c^*\right]_{r^*=1} = 0, \tag{6}$$

$$\text{also at} \quad z^* = 0 \quad \frac{\partial c^*}{\partial z^*} = 0, \tag{7}$$

and at $z^*=1^*$ $$\left[\frac{\partial c^*}{\partial z^*}+\frac{\alpha R}{D}c^*\right]_{z^*=1^*}=0. \tag{8}$$

By definition, the dimensionless Sherwood number is: $\alpha d/D$ (where $d = 2R$). Hence, boundary conditions in eqn (6) and eqn (8) can be written as

$$\left[\frac{\partial c^*}{\partial r^*}+\frac{Sh}{2}c^*\right]_{r^*=1}=0, \tag{9}$$

$$\left[\frac{\partial c^*}{\partial z^*}+\frac{Sh}{2}c^*\right]_{z^*=l^*}=0. \tag{10}$$

Finite difference model

The finite difference method was applied in a given calculation area to approximate function derivatives at a point from values at several neighbouring points (Fig. 1). To solve such problem, the ADI method was used. This method is based on two different finite difference equations, one implicit only in the radial direction and the other one implicit only in the axial direction, and was applied over successive time intervals of duration $\Delta t/2$.

First stage. eqn (2) was discretized in the z direction. The value of j was fixed and i was varied from 1 to $i_{\max}$ for the first half time intervals of $t+\Delta t/2$. This time step is markedly n'.

$$\frac{c^{*n'}_{i,j}-c^{*n}_{i,j}}{\Delta t^*/2}=\frac{c^{*n'}_{i-1,j}-2c^{*n'}_{i,j}+c^{*n'}_{i+1,j}}{\Delta z^{*2}}+\frac{c^{*n}_{i,j-1}-2c^{*n}_{i,j}+c^{*n}_{i,j+1}}{\Delta r^{*2}}$$
$$+\frac{1}{r^*}\,\frac{c^{*n}_{i,j+1}-c^{*n}_{i,j-1}}{2\Delta r^*}. \tag{11}$$

Rearrangement of eqn (11) results in

$$\left(\frac{1}{\Delta z^{*2}}\right)c^{*n'}_{i-1,j}+\left(-\frac{2}{\Delta t^*}-\frac{2}{\Delta z^{*2}}\right)c^{*n'}_{i,j}+\left(\frac{1}{\Delta z^{*2}}\right)c^{*n'}_{i+1,j}$$

$$=\left(-\frac{1}{\Delta r^{*2}}+\frac{1}{2r^*\Delta r^*}\right)c^{*n}_{i,j-1}+\left(\frac{2}{\Delta r^{*2}}-\frac{2}{\Delta t^*}\right)c^{*n}_{i,j}$$

$$+\left(-\frac{1}{\Delta r^{*2}}+\frac{1}{2r^*\Delta r^*}\right)c^{*n}_{i,j+1}. \tag{12}$$

By discretizing the boundary conditions in eqns (7) and (10), the following was obtained:

$$\frac{\partial c^*}{\partial z^*}=0 \Rightarrow \frac{c^{*n'}_{2,j}-c^{*n'}_{1,j}}{\Delta z^*}=0 \Rightarrow c^{*n'}_{2,j}=c^{*n'}_{1,j}, \tag{13}$$

$$\left[\frac{\partial c^*}{\partial z^*}+\frac{Sh}{2}c^*\right]_{z^*=l^*}=c^* \Rightarrow c^{*n'}_{i_{\max},j}=\frac{c^{*n'}_{i_{\max-1},j}}{1-(Sh\Delta z^*/2)}. \tag{14}$$

By varying i from 2 to $i_{\max-1}$ and introducing eqn (13) and eqn (14) into eqn (12) a system of $i_{\max-1}$ equations and $i_{\max-1}$ unknowns was obtained.

$$\mathbf{A}\boldsymbol{x}=\boldsymbol{b}, \tag{15}$$

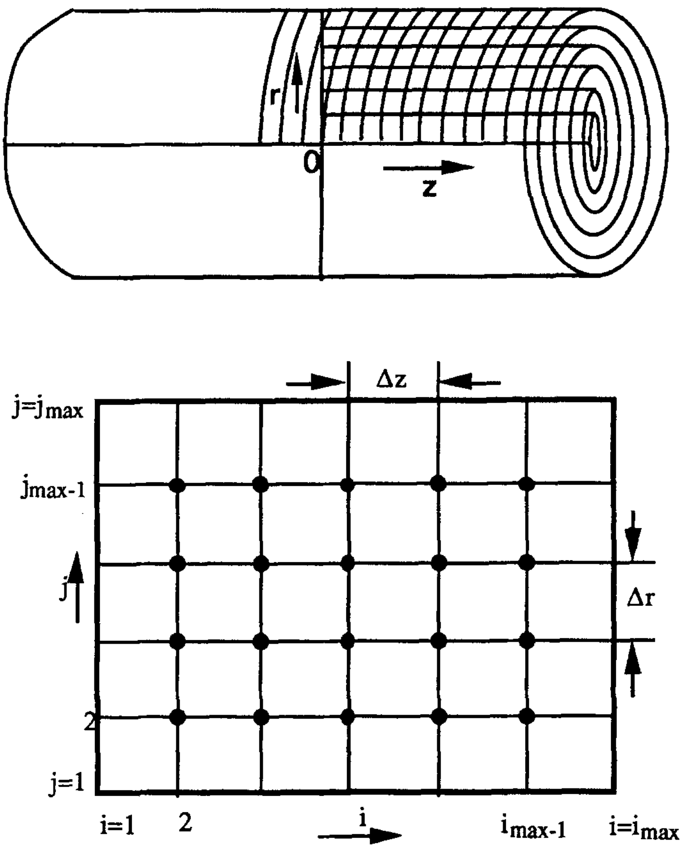


Fig. 1. Arrangement of mesh points in a cylinder for the finite difference scheme to predict volatile migration. Δr and Δz represent the vertical and horizontal distance between the nodes.

$$
A=\begin{bmatrix}
D(i=2) & C(i=2) & & & \\
A(i=3) & D(i=3) & C(i=3) & & \\
 & \ddots & \ddots & \ddots & \\
 & & A(i_{\max}-2) & D(i_{\max}-2) & C(i_{\max}-2) \\
 & & & A(i_{\max}-1) & D(i_{\max}-1)
\end{bmatrix}
$$

$$
\boldsymbol{x}=\begin{bmatrix} c^{*n'}_{2,j} \\ c^{*n'}_{2,j} \\ \vdots \\ c^{*n'}_{i_{\max}-1,j} \end{bmatrix} \text{ and } \boldsymbol{b}=\begin{bmatrix} b_{2,j} \\ b_{3,j} \\ \vdots \\ b_{i_{\max}-1,j}\end{bmatrix}.
$$

In this equation set $\boldsymbol{A}$ is the matrix of coefficients, $\boldsymbol{x}$ is the vector of concentrations at an intermediate time to be calculated and $\boldsymbol{b}$ is the vector of concentrations of initial time. Where

$$
D(i=2)=\frac{1}{\Delta z^{*2}}-\frac{2}{\Delta t^{*}}-\frac{2}{\Delta x^{*2}},\quad D(i)=\frac{-2}{\Delta t^{*}}-\frac{2}{\Delta z^{*2}},
$$

$$
D(i_{\max}-1)=\frac{-2}{\Delta t^{*}}-\frac{2}{\Delta z^{*2}}+\frac{1}{\Delta z^{*2}(1+Sh\Delta z^{*}/2)},\quad A(i)=\frac{1}{\Delta z^{*2}},\quad C(i)=\frac{1}{\Delta z^{*2}},
$$

$$
B(i)=\left(\frac{-1}{\Delta r^{*2}}+\frac{1}{2r^{*}\Delta r^{*}}\right)c^{*n}_{i,j-1}+\left(\frac{2}{\Delta r^{*2}}-\frac{2}{\Delta t^{*}}\right)c^{*n}_{i,j}
$$

$$
+\left(-\frac{1}{\Delta r^{*2}}-\frac{1}{2r^{*}\Delta r^{*}}\right)c^{*n}_{i,j+1}. \tag{16}
$$

Second stage. eqn (3) was to be discretized for fixed i and variable j from 1 to $j_{\max}$, for the second half time interval as follows:

$$
\frac{c^{*n+1}_{i,j}-c^{*n'}_{i,j}}{\Delta t^{*}/2}=\frac{c^{*n'}_{i-1,j}-2c^{*n'}_{i,j}+c^{*n'}_{i+1,j}}{\Delta z^{*2}}+\frac{c^{*n+1}_{i,j-1}-2c^{*n+1}_{i,j}+c^{*n+1}_{i,j+1}}{\Delta r^{*2}}
$$

$$
+\frac{1}{r^{*}_{i,j}}\,\frac{c^{*n+1}_{i,j+1}-c^{*n+1}_{i,j-1}}{2\Delta r^{*}}. \tag{17}
$$

Discretizing eqns (5) and (9), results in eqns (18) and (19).

$$
c^{*n+1}_{i,1}=c^{*n+1}_{i,2}, \tag{18}
$$

$$
c^{*n+1}_{i,j_{\max}}=\frac{c^{*n+1}_{i,j_{\max}-1}}{1+(\Delta r^{*}Sh/2)}. \tag{19}
$$

Introducing these boundary conditions in eqn (17) for 'j' from 2 to $j_{\max-1}$, another system of equations of $j_{\max-1}$ equations and $j_{\max-1}$ unknowns as obtained.

$$
\boldsymbol{A'x'}=\boldsymbol{b'} \tag{20}
$$

where A' is the matrix of coefficients; x' is the vector of concentrations at complete time interval which is to be calculated and b' is the vector of concentrations at intermediate time which has been calculated in the first stage.

To solve these systems of equations, the Gaussian elimination method was applied. A computer program, Tridiagonal Matrix Algorithm (TDMA), was used to solve equation sets (Fig. 2). Numerical output of this program was introduced to Matlab® software which permitted the plotting of graphical presentations of the mathematical models.

Experimental

Volatile constituents of wooden packaging

The volatile molecules present in wooden packaging samples were identified by MS Fisons TRIO 1000 (column DB5MS 15 m, 0·32 mm, 0·25 μm and Gaz vector He C) coupled with GC (Teckmar). Benzaldehyde was detected as an important volatile constituent of wooden samples (Fig. 3).

Benzaldehyde diffusivity in agar gel

The diffusivity of Benzaldehyde was determined according to the method described by Belton and Wilson (1982) which consists of measuring concentrations of diffusing substance along an insulated cylinder, for different positions and times. A long insulated cylinder (140 mm high and 6 mm radius) of agar gel was let interdiffuse with diluted benzaldehyde solution in water (0·3%). The cylinder was positioned vertically at the solution surface in a 50 ml ballon at 20°C. Diffusant concentrations, diffused in the axial direction, at different cylinder heights and different times were measured by head space gas chromatography (HSGC model 8500 Perkin–Elmer & Co GmbH, Äberlingen, Germany).

The diffusion coefficient was calculated by means of theoretical curves of a dimensionless model (Fig. 4) which was developed by application of the numerical solution of the axial diffusion problem in a finite cylinder

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{21}$$

with the initial condition $t=0$, $c=0$ and boundary conditions $t>0$; $x=0$, $c=c_o$et $x=L$, $\partial c/\partial x=0$.

The explicit method of finite difference equations to solve eqn (21) requires the introduction of the following dimensionless parameters:

$$C=\frac{c-c_o}{-c_o}\ t^*=\frac{tD}{L^2}\ x^*=\frac{x}{L}.$$

Introducing the above parameters to eqn (21), results in

$$\frac{\partial C}{\partial t^*} = \frac{\partial^2 C}{\partial x^{*2}}. \tag{22}$$

By discretizing eqn (22), the following was obtained:

$$\frac{C_{i,n+1}-C_{i,n}}{\Delta t^*} = \frac{C_{i-1,n}-2C_{i,n}+C_{i+1,n}}{\Delta x^{*2}}. \tag{23}$$

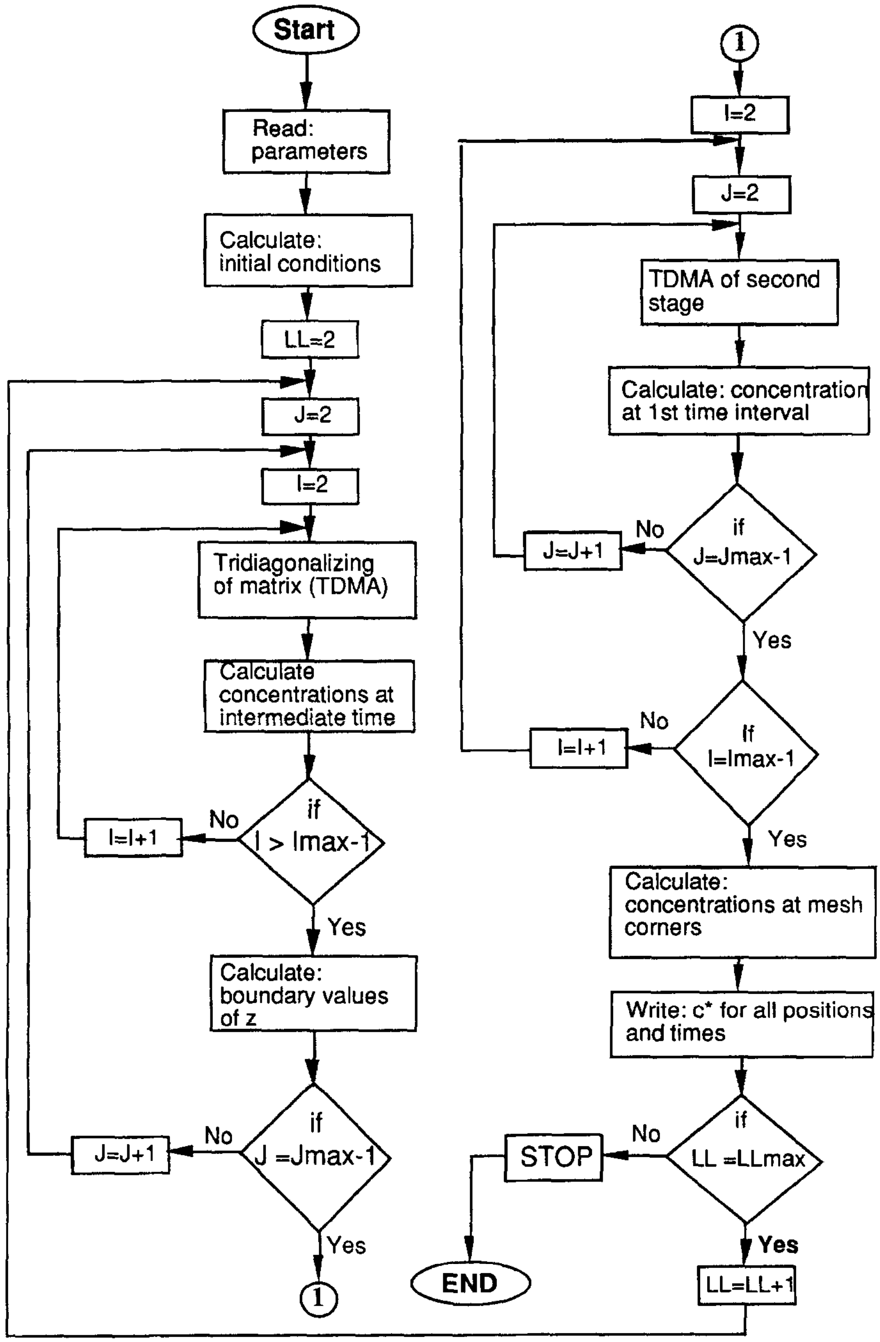


Fig. 2. Flow diagram of the computer program for two-dimensional transient mass transfer in a cylindrical shape.

Rearranging eqn (23) resulted in eqn (24) which was solved by a computer program (Fortran 77).

$$C_{i,n+1} = \left(\frac{\Delta t^*}{\Delta x^{*2}}\right)C_{i-1,n} + \left(1 - \frac{2\Delta t^*}{\Delta x^{*2}}\right)C_{i,n} + \left(\frac{\Delta t^*}{\Delta x^{*2}}\right)C_{i+1,n}. \tag{24}$$

Numerical results of this program were treated by a Matlab program which permitted the plotting of the theoretical curves.

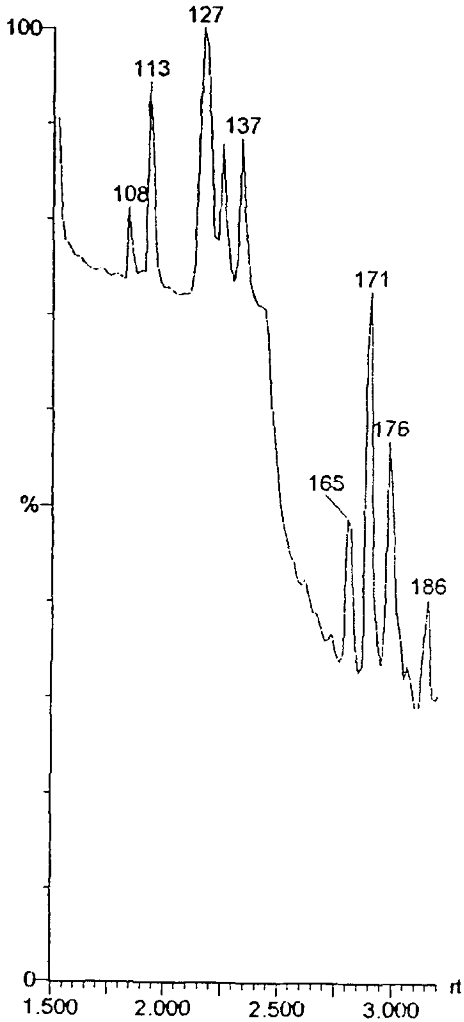


Fig. 3. Mass spectrometry for detection of volatile compounds of wood package. Peak 176 is related to benzaldehyde.

Knowing the results derived from experimental measurement of concentrations of the diffusant at various times and positions of the cylinder, these curves (Fig. 4) allowed the calculation of the diffusion coefficient. The average benzaldehyde diffusion coefficient, derived from 50 experiments was $1{\cdot}1 \times 10^{-6} \pm 0{\cdot}1 \times 10^{-6}$ cm^2 s^{-1}.

Benzaldehyde partition coefficient

The partition coefficient of benzaldehyde was determined according to the method applied by Halek and Hatzidimitriu (1988), by equilibrating several quantities of benzaldehyde solution with the material studied. The partition coefficient was determined between package and free space air and also between a cylindrical agar gel and air. This was in a 9 ml closed vial (Tables 1 and 2). Equilibration was complete at 20°C after 2 days. The benzaldehyde concentration was measured by HSGC.

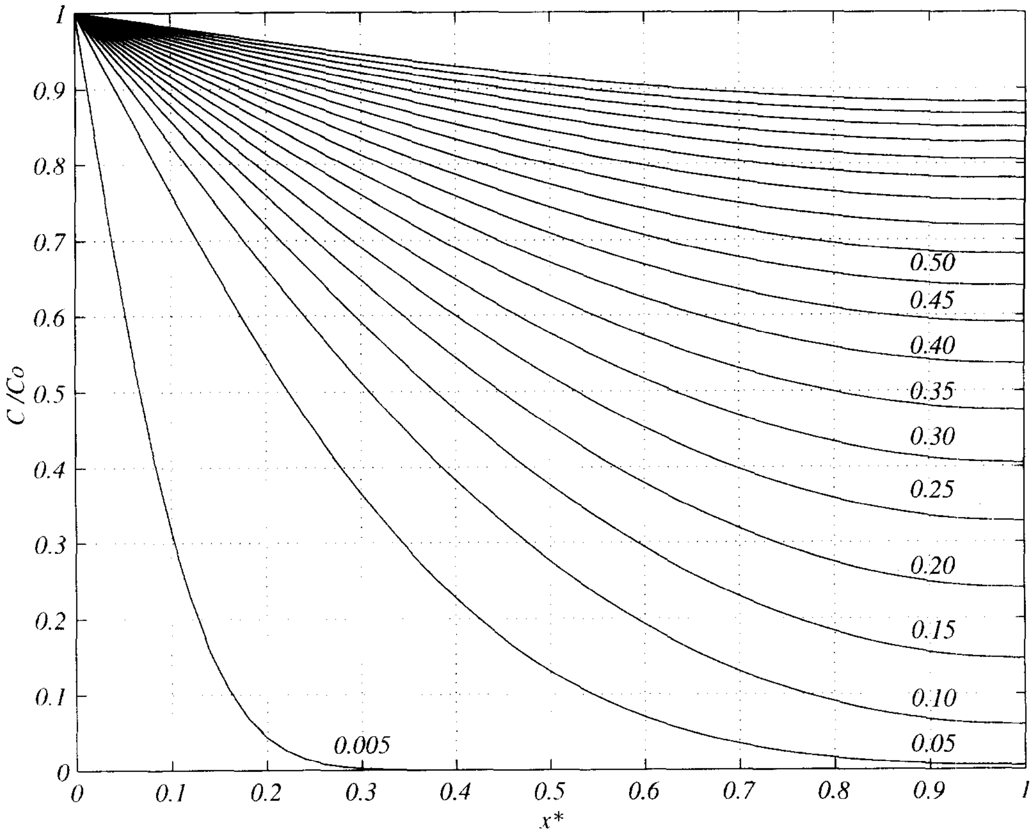


Fig. 4. Theoretical curves to determine diffusion coefficient, generated by computerized numerical solution of axial diffusion in a finite cylinder. Numbers on the curves are dimensionless times ($t^* = tD/L^2$). Where t is the diffusion time (s); D is the diffusion coefficient of diffusant in gel cylinder; x^* is the normalized height of cylinder; C is the concentration of diffusant; C_o is the initial concentration of diffusant at the interdiffusing point of cylinder; L is the height of cylinder (cm).

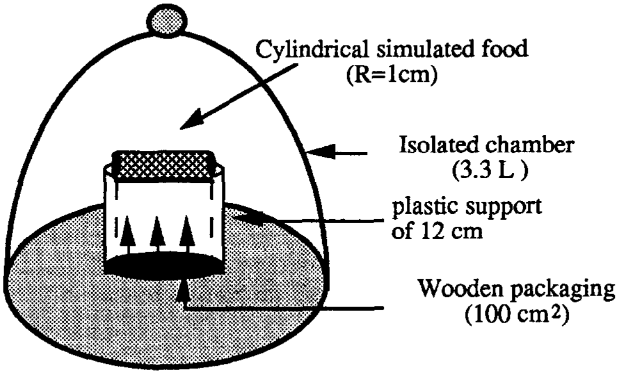


Fig. 5. Assembling of package simulating chamber.

TABLE 1
Partition Coefficient Between Agar Gel Cylinder and Air

C_i	C_g	C_a	K_p
0·1	0·425	1·5	0·283
0·2	0·873	2·533	0·344
0·3	1·338	3·236	0·413
0·4	1·771	4·561	0·388
0·5	2·227	5·445	0·408
0·6	2·680	6·397	0·419
0·7	3·113	7·724	0·403
0·8	3·568	8·622	0·413
0·9	4·007	9·843	0·407
1·0	4·443	11·337	0·391

TABLE 2
Partition Coefficient Between Package Wood and Air

C_i	C_w	C_a	K_p
0·6	11·689	3·246	3·601
0·7	14·293	3·546	4·030
0·8	16·03	3·875	4·204
0·9	17·610	4·556	3·865
1	18·415	5·087	3·619

C_i = Benzaldehyde quantity (μg) injected initially in vial; C_w = μg benzaldehyde per g of wood; C_a = μg benzaldehyde per g of air; C_g = μg benzaldehyde per g of agar gel; K = partition coefficient.

Packaging simulating chamber
In a 3.3 liter enclosure, benzaldehyde migration was permitted to happen between a wood sheet and a cylindrical shape agar gel (Biokar, Beauvais, France). The gel was held on a support of 12 cm height (Fig. 5). For various times and positions of the cylinder (100 mm high and 20 mm radius), the benzaldehyde concentration was measured, by HSGC, to verify the mathematical model. Temperature was maintained at 20°C for all experiences.

RESULTS AND DISCUSSION

The experimental method was applied to determine the diffusivity of volatile compounds in agar gel. This method which has been widely used by different authors was improved in this study to simplify calculating of diffusion coefficient (Fig. 4).

Theoretical curves with a different non-dimensional time parameter and also non-dimensional parameters on the *yx*-axis permit the calculation of the diffusivity in a simple way. Numbers on the curves are non-dimensional times ($t^* = tD/L^2$) where t is the diffusion time (s); D is the diffusion coefficient of diffusant substance to be calculated ($m^2 s^{-1}$) and L is the length of the cylinder. From the normalized concentration (C/C_o) versus normalized length of the cylinder can be found the related position of non-dimensional times, which provides the calculation of 'D'.

Partition coefficient values and benzaldehyde diffusivity in agar gel, applied in model validation, were likely to be precisely mesured. There was a relationship between C_o and C_w since $C_o = C_w/10$.

The computer program developed in this paper was able to solve two-dimensional transient diffusion in a cylinder with convective boundary conditions by the finite difference numerical method and a Matlab program presented numerical outputs in 3-D models. Figure 6 shows concentration profiles in both the radial and axial direction of the cylinder, for different dimensionless times (t^*). At both extremities of the cylinder, migrant concentration is at its highest level due to two-dimensional diffusion. For the model, the Sherwood number was fixed at 0·36, according to Chilton–Colbern analogy (Saatdjian, 1993), which describes *Nu* and *Sh* as analogs to heat and mass transfer. Bejan (1995) described *Nu* (Nusselt number) with the following equation:

$$Nu_D = \left\{0\cdot6 + \frac{0\cdot387 Ra_D^{1/6}}{[1+(0\cdot559/Pr)^{9/16}]^{8/27}}\right\}^2. \qquad (25)$$

When the Raleigh number (analog to Reynolds number) tends toward zero, *Nu* is nearly 0·36. Experimental data showed that such a *Sh* value defined well the boundary conditions of a packaged cylinder which is subjected to volatile constituent migration from packaging material through surrounding air (natural convection at the boundaries). Benzaldehyde concentrations ($\mu g\ g^{-1}$) in the simulated food were measured at various times and compared with those of models. This confirmed the use of the Chilton–Colbern analogy of heat and mass transfer and *Sh* value (0·36) for such cases. The model closely simulated transient two-dimensional diffusion of benzaldehyde into a cylindrical shaped food analogous to (Figs 7–9). Good agree-

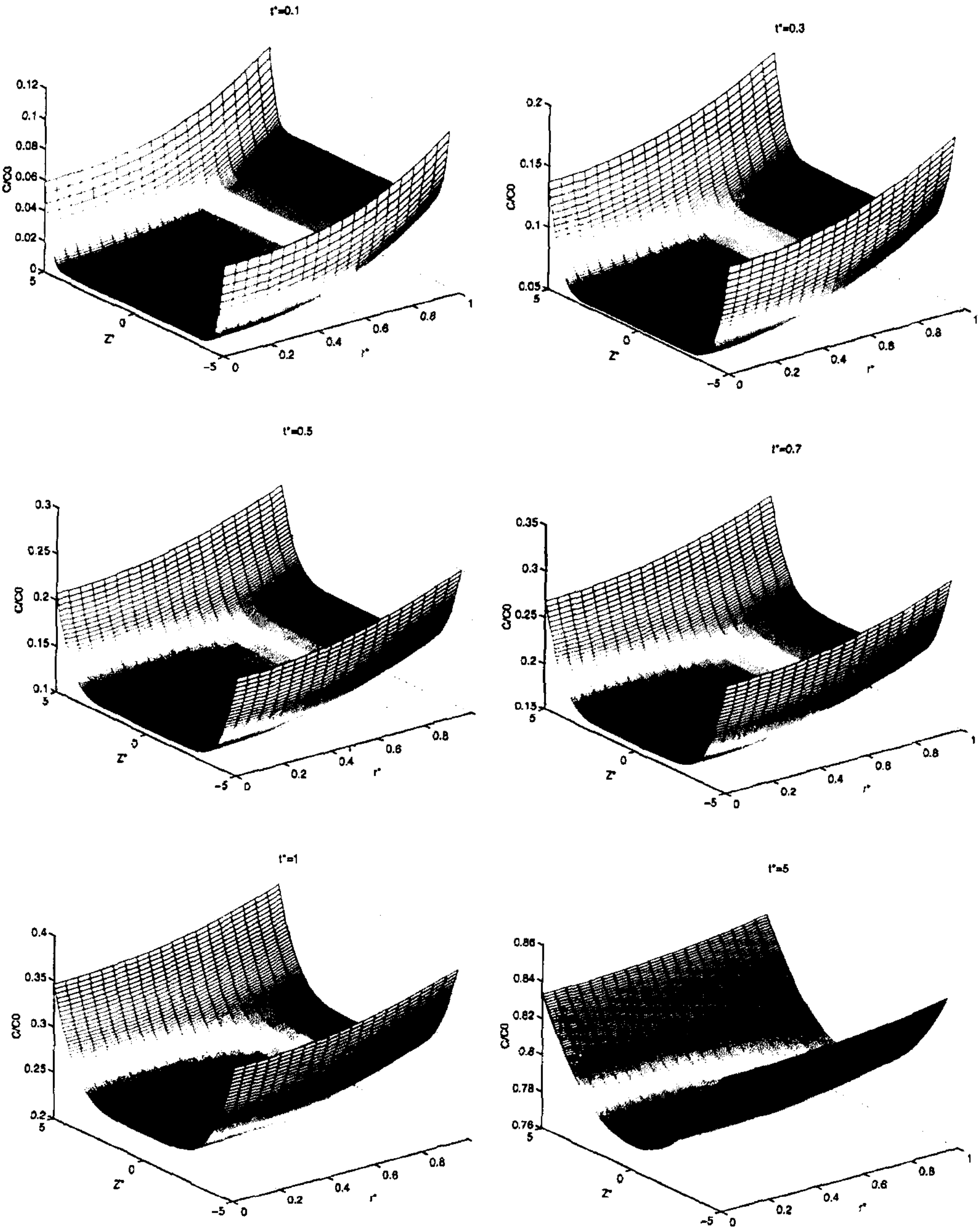
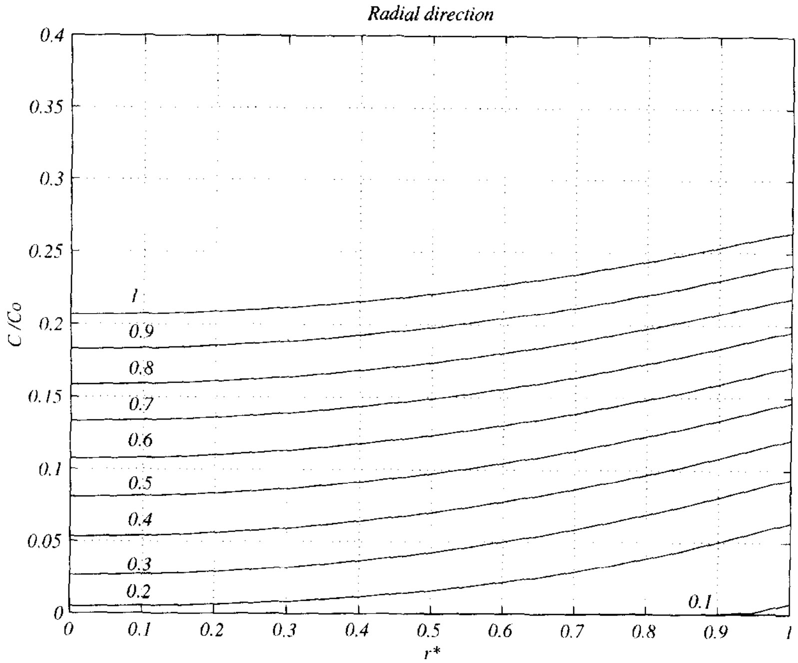


Fig. 6. Predictive models of volatile migration in packaged cylindrical shape for different dimensionless times ($t^* = tD/R^2$). Where t is the diffusion time (s), D is the diffusivity of volatile compound in packaged material ($cm^2\,s^{-1}$) and R is the cylinder radius (cm); (b) predictive models of radial and axial diffusion in a cylinder. Normalized concentration is plotted versus normalized radius and normalized axis. Numbers on the curves are dimensionless times (t^*).



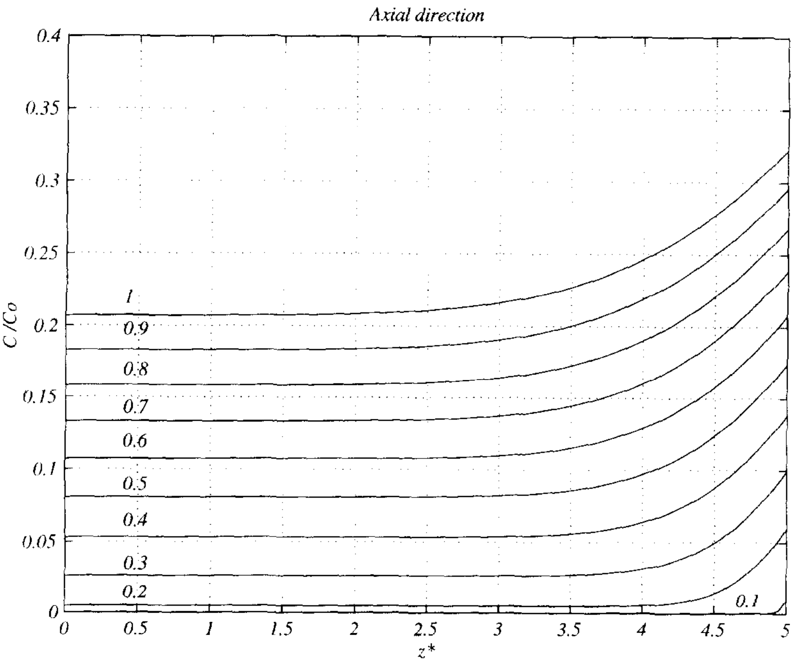


Fig. 6. *Continued*

ment was observed between experimental and theoretical results derived from the mathematical model. Although mass transfer by convection in food packaging is not as important as diffusion generated by wrapping foodstuffs in package materials, such migration of volatile constituents may be interesting in formulation of legislation. Wood packaging has not yet been considered as a resource which can liberate volatile constituents. Therefore no research has been reported to investigate migration from this kind of package or container in food processing or food packaging. This paper demonstrates the efficiency of mathematical models of migration even for the cases with apparently less importance in food packaging.

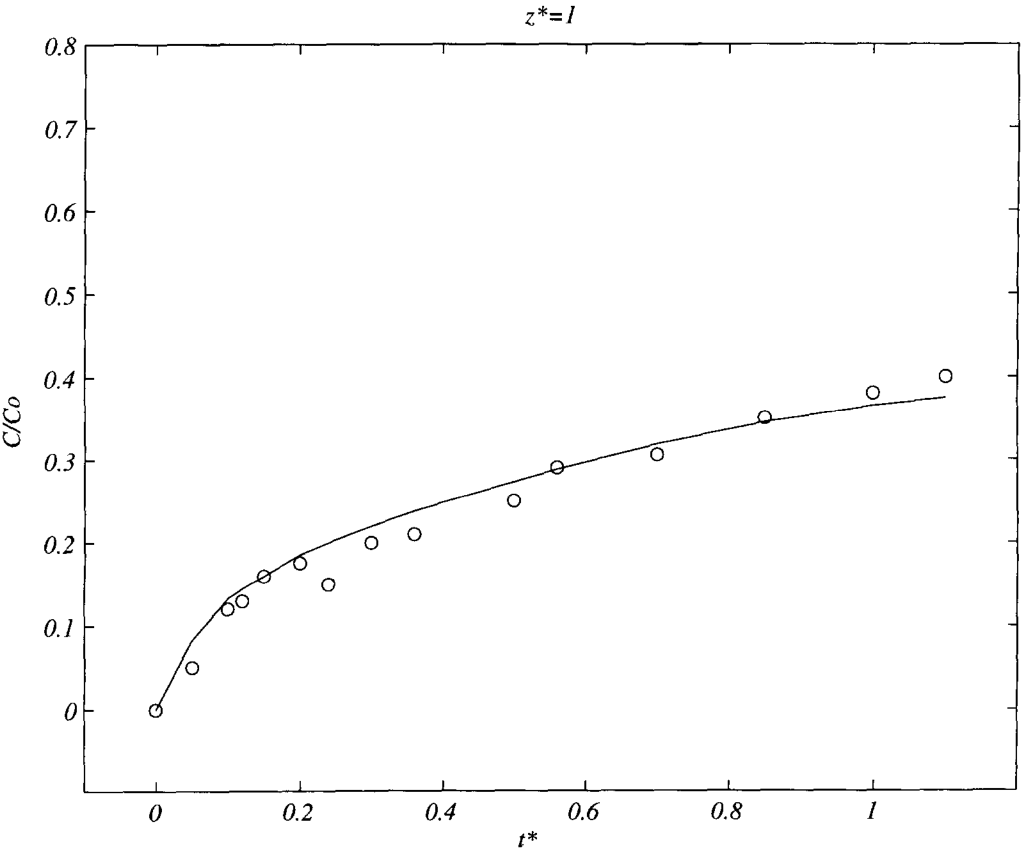


Fig. 7. Migrant concentration profile at cylinder extremity, generated by measurement of migrated volatile compounds from simulated packaging material to simulated food via package free space at 20°C (———, best-fit curve using data obtained by numerical solution of two-dimensional diffusion in a finite cylinder, ○, experimental data). Normalized concentration is plotted versus dimensionless time (t^*).

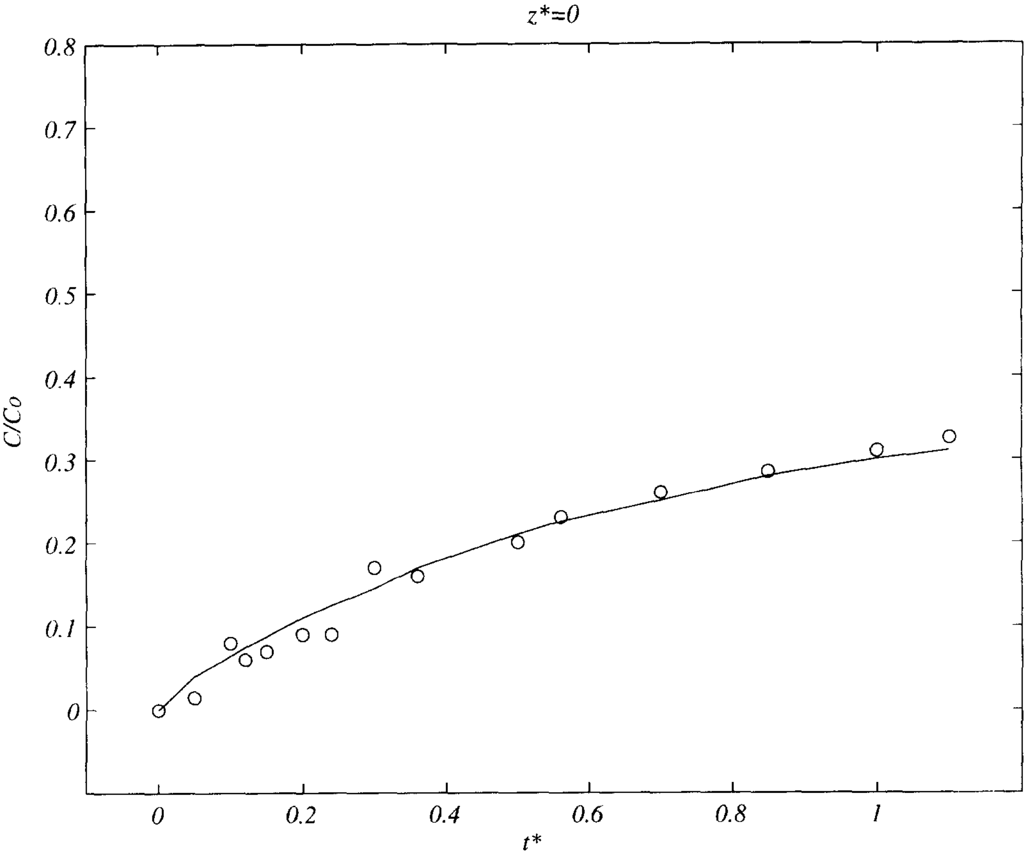


Fig. 8. Migrant concentration curve in center of cylinder, generated by measurement of migrated volatile compounds from simulated packaging material to simulated food via package free space at 20°C (———, best-fit curve using data obtained by numerical solution of two-dimensional diffusion in a finite cylinder; ○, experimental data).

CONCLUSION

The models developed in this study predicted concentration distribution of volatile molecules during packaged food storage. The model can be used for a great range of homogeneous food products. Numerical solutions applied in this study are likely to be effective for such diffusion problems even for more complex geometries and sophisticated boundary conditions. However, application of this model is limited to cases governed by convection at the boundaries. Similar mass transfer as studied in this paper has not been sufficiently studied for migration phenomenon in food packaging.

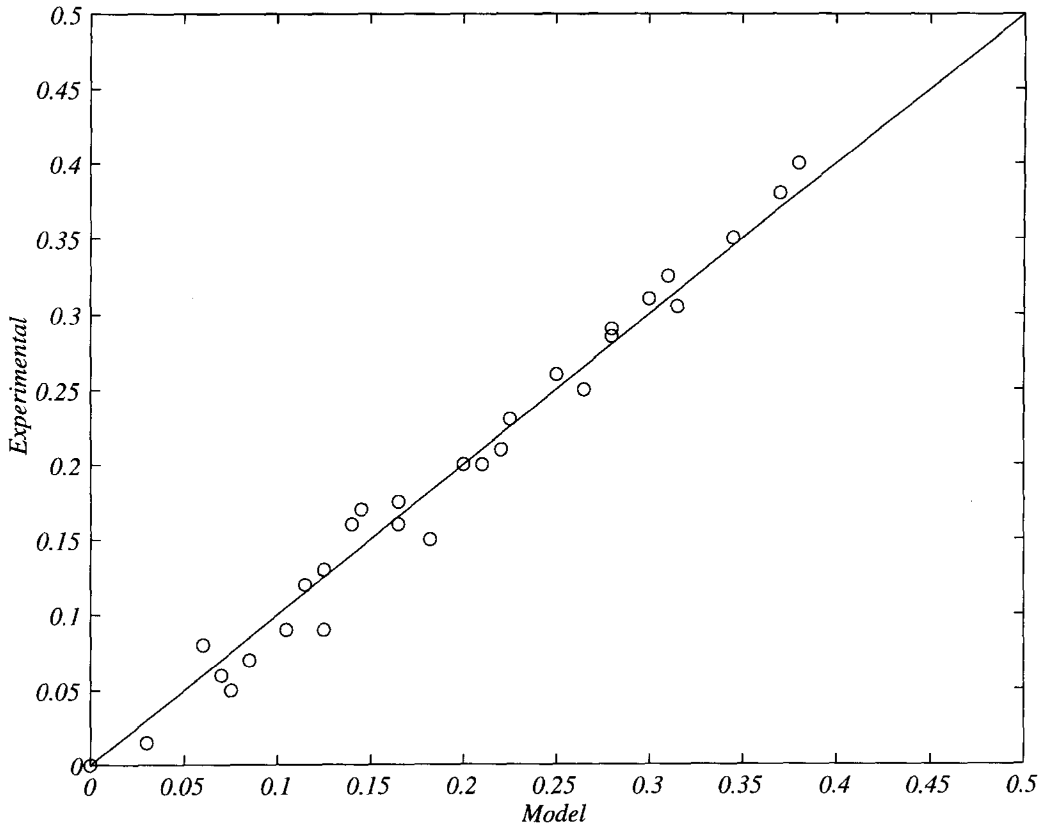


Fig. 9. Model validation, confirmed by agreement between theoretical (derived from numerical solution of diffusion in a finite cylinder) and experimental data.

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