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# AN APPROXIMATE METHOD FOR THE NONLINEAR DIFFUSION PROBLEM WITH A POWER RELATION BETWEEN DIFFUSION COEFFICIENT AND CONCENTRATION—I. COMPUTATION OF DESORPTION TIMES

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**Abstract**—A method is proposed for approximate calculations, concerning concentration dependent diffusion with a power relation between diffusion coefficient and concentration ($D_r = m^a$). This method can be applied to a desorption process in non-shrinking or shrinking systems with slab, cylindrical or spherical geometry. The method is developed for desorption with a uniform initial concentration profile and Dirichlet boundary conditions, i.e. constant surface concentration and symmetry with respect to the centre, central axis or central plane of the system. The method can ultimately be used for predicting the time behaviour of average concentration and flux, resulting in accurate approximations to the exact solutions, obtained by analytical or numerical techniques.

## NOMENCLATURE

| | |
|---|---|
| $a$, | power in concentration dependence of diffusion coefficient; |
| $B, B_x$, | beta function, incomplete beta function; |
| $d$, | density [kg/m$^3$]; |
| $D$, | diffusion coefficient [m$^2$/s]; |
| $E$, | efficiency desorption process; |
| $f$, | time dependent part of the particular solution of the diffusion equation; |
| $F$, | flux parameter; |
| $g$, | space dependent part of the particular solution of the diffusion equation; |
| $G$, | flux function; |
| $H$, | shrinkage factor; |
| $j$, | mass flux [kg/m$^2$ s]; |
| $m$, | dimensionless concentration; |
| $n$, | mass flux [kg/m$^2$ s]; |
| $r$, | space coordinate [m]; |
| $R$, | radius or half-thickness of the system [m]; |
| $Sh_d$, | average Sherwood number of the dispersed phase; |
| $t$, | time [s]; |
| $X$, | geometry variable. |

Greek symbols

| | |
|---|---|
| $v$, | geometry parameter; |
| $\phi$, | dimensionless space coordinate; |
| $\rho$, | mass concentration [kg/m$^3$]; |
| $\tau$, | dimensionless time. |

Subscripts

| | |
|---|---|
| c, | centre; |
| i, | interface; |
| m, | migrating component; |
| o, | initial; |
| $Q$, | referring to inflection point $Q$; |
| r, | reduced; |
| s, | non-diffusing reference component; |
| $S$, | refers to maximum $S$. |

Superscripts

| | |
|---|---|
| $\bar{}$, | average value; |
| $*$, | referring to shrinking systems; |
| $^{(n)}$, | $n$th derivative. |

## 1. INTRODUCTION

THE USUAL approach for solving nonlinear diffusion problems is the application of numerical techniques, which as a rule are only suitable for high-speed large-memory computers and require the necessary programming skill. In practice it would therefore be convenient when approximate methods, based on straightforward computational procedures are available for this class of problems in order to avoid time consuming programming and computing.

This paper is concerned with the construction of such a computational procedure for desorption in non-shrinking or shrinking slabs, cylinders and spheres, which does not involve numerical techniques to solve the nonlinear partial differential equation describing the diffusion process. Although the method developed here is restricted to diffusion coefficients which are power functions of the concentration, this specific case is one of considerable interest for nonlinear diffusion in porous media, a topic which has received much attention in mathematical analysis in the last ten years, due to its importance in oil engineering and hydrology [1–7]. Other fields of possible applications are diffusion of vapours in highpolymer substances [8], drying of porous materials [9–11] and nonlinear heat diffusion in metals as aluminium and iron [12]. Furthermore, the approximate method is restricted to desorption with a uniform initial concentration profile and Dirichlet boundary conditions, also known as boundary conditions of the first kind.

Other approximate methods were reported by Suzuki *et al.* [9], who developed a model for low-intensity drying of slabs, based on the assumption of a pseudo steady state, and by Schoeber [10, 11], who introduced a general method for a short-cut calculation of the mass flux in nonlinear diffusion problems. The basic concept of Schoeber's method is the combination of the "short time solution", usually referred to as the penetration period, and the "large time solution", referred to as the regular regime.

The same concept of combining these two limiting solutions served as a basis for this paper, although the transition between the two solutions, as well as the effect of shrinkage were approached in a different way.

An analysis of the numerical solution resulted in a simplified model for the specific case of nonlinear diffusion, mentioned above. The computational procedure involved merely consists of a sequence of straightforward calculations resulting in desorption times for non-shrinking or shrinking slabs, cylinders and spheres.

In the following sections we shall be concerned with the formulation of the nonlinear diffusion problem (section 2) and the construction of the approximate method for non-shrinking and shrinking systems, treated separately (section 3). Finally, in section 4, a comparison is made between the results obtained by the approximate method and those obtained by solving the partial differential equation by a finite differences technique.

An extension of the present approximate method, concerning the computation of the concentration profiles during the desorption process will be treated in a supplementary paper [16].

## 2. THE NONLINEAR DIFFUSION PROBLEM

### 2.1. *The diffusion equation*

A generalized formulation of the diffusion equation [10] is expressed by the following relation:

$$\frac{\partial m}{\partial \tau} = \frac{\partial}{\partial \phi}\left(D_r X^2 \frac{\partial m}{\partial \phi}\right) \tag{1}$$

which holds for concentration dependent diffusion in non-shrinking and shrinking slabs, cylinders and spheres. Before proceeding we shall first define the dimensionless variables, occurring in equation (1) for non-shrinking and shrinking systems, respectively.

2.1.1. *Non-shrinking systems.* For non-shrinking systems a stationary coordinate system can be applied in which the dimensionless concentration $m$ is defined as

$$m = \frac{\rho_m}{\rho_{m,o}} \tag{2}$$

with $\rho_m$ the mass concentration of the migrating component at time $t$ and $\rho_{m,o}$ the initial mass concentration.

The dimensionless time $\tau$ is defined as

$$\tau = \frac{D_o t}{R^2}, \tag{3}$$

where $D_o$ represents a reference value of the diffusion coefficient and $R$ the radius or half-thickness of the system.

The dimensionless space coordinate $\phi$ is defined as

$$\phi = \left(\frac{r}{R}\right)^{v+1} \tag{4}$$

with $r$ the space coordinate and $v$ a geometry parameter, having the values 0, 1 and 2 for slab, cylinder and sphere, respectively.

The dimensionless diffusion coefficient $D_r$ is defined as

$$D_r = \frac{D}{D_o} \tag{5}$$

with $D$ the diffusion coefficient.

Finally, the dimensionless geometry variable $X$ is defined as

$$X = (v+1)\phi^{v/(v+1)}. \tag{6}$$

2.1.2. *Shrinking systems.* For shrinking systems the application of a reference component mass centered coordinate system avoids the complication of a moving boundary [13]. In this coordinate system the dimensionless concentration $m$ is now defined as

$$m = \left(\frac{\rho_m}{\rho_s}\right) \Big/ \left(\frac{\rho_{m,o}}{\rho_{s,o}}\right) \tag{7}$$

with $\rho_s$ the mass concentration of a non-diffusing reference component $s$. If the density of this reference component does not change upon mixing, the dimensionless time $\tau$ can be defined as

$$\tau = \frac{D_o \rho_{s,o}^2}{d_s^2 R_s^2} t \tag{8}$$

with $\rho_{s,o}$ the initial mass concentration of reference component $s$, $d_s$ the density of the reference component and $R_s$ the radius or half-thickness of the system in case the mass concentration of the reference component would be equal to its density. This so-called "dry solids radius" $R_s$ is related to the initial radius $R_o$ of the system by

$$R_s = \left(\frac{\rho_{s,o}}{d_s}\right)^{1/(v+1)} R_o. \tag{9}$$

The dimensionless space coordinate $\phi$ is now defined as

$$\phi = \int_0^r \rho_s r^v \,\mathrm{d}r \Big/ \int_0^R \rho_s r^v \,\mathrm{d}r =$$

$$= \frac{\nu + 1}{\rho_{s,o} R_o^{\nu+1}} \int_0^r \rho_s r^\nu \, \mathrm{d}r. \tag{10}$$

The dimensionless diffusion coefficient is defined as

$$D_r = \frac{D \rho_s^2}{D_o \rho_{s,o}^2} \tag{11}$$

and the dimensionless geometry variable $X$ as

$$X = (\nu + 1) \left\{ \int_0^\phi \left( 1 + \frac{d_s \rho_{m,o}}{d_m \rho_{s,o}} m \right) \mathrm{d}\phi \right\}^{\nu/(\nu+1)} \cdot \tag{12}$$

### 2.2. *Initial and boundary conditions*

The generalized formulation for the diffusion equation has to be applied to the initial and boundary conditions as well. In this paper we restrict ourselves to Dirichlet boundary conditions (boundary conditions of the first kind) and the initial condition of a uniform initial concentration profile. This set of conditions in dimensionless form then reads:

$$m = m_o = 1 \quad \text{for } \tau = 0 \quad \text{and } 0 \leqq \phi \leqq 1 \tag{13}$$

$$X \frac{\partial m}{\partial \phi} = 0 \quad \text{for } \tau > 0 \quad \text{and } \phi = 0 \tag{14}$$

$$m = m_i = 0 \quad \text{for } \tau > 0 \quad \text{and } \phi = 1. \tag{15}$$

## 3. AN APPROXIMATE METHOD FOR THE COMPUTATION OF THE MASS FLUX AND DESORPTION TIME

### 3.1. *Non-shrinking systems*

For the nonlinear diffusion equation with $D_r = m^a$, no explicit general solution in terms of known functions could be derived analytically. For a slab, however, a particular solution exists, which represents the "large time solution", but is only applicable when the centre concentration starts to deviate appreciably from the initial centre concentration (regular regime). By putting $m(\phi, \tau) = f(\tau) g(\phi)$, this particular solution can be found after separation and subsequent solution of the space and time dependent parts. The derivation of this particular solution will not be given here, but will be accommodated in a supplementary paper [16]. When we assume the regular regime to be valid at time $\tau_Q$, when the average concentration has arrived at a value $\bar{m}_Q$, the particular solution reads:

$$m(\phi, \tau) = \frac{1}{2} B\left(\frac{a+1}{a+2}, \frac{1}{2}\right) g_r(\phi) \left[ \bar{m}_Q^{-a} + \frac{a}{a+2} \times \frac{1}{2^{a+1}} B^{a+2}\left(\frac{a+1}{a+2}, \frac{1}{2}\right)(\tau - \tau_Q) \right]^{-1/a} \tag{16}$$

with

$$g_r(\phi) = \frac{g(\phi)}{g(0)} = \frac{g(\phi)}{g_c} \tag{17}$$

which follows from the implicit equation:

$$B_z\left(\frac{a+1}{a+2}, \frac{1}{2}\right) = B\left(\frac{a+1}{a+2}, \frac{1}{2}\right)(1 - \phi) \quad \text{with } z = g_r^{a+2}. \tag{18}$$

The functions $B$ and $B_z$ represent the beta and incomplete beta function, respectively [14, 15]. They can be expressed by infinite series, according to

$$B_z\left(\frac{a+1}{a+2}, \frac{1}{2}\right) = \left(\frac{a+2}{a+1}\right) \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n}(n!)^2} \frac{z^{n+(a+1)/(a+2)}}{n\left(\frac{a+2}{a+1}\right) + 1} \tag{19}$$

and

$$B\left(\frac{a+1}{a+2}, \frac{1}{2}\right) = \left(\frac{a+2}{a+1}\right) \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n}(n!)^2} \frac{1}{n\left(\frac{a+2}{a+1}\right) + 1}. \tag{20}$$

The average value of $g_r$ follows from integration by parts of equation (18) (see Appendix A), resulting in

$$\bar{g}_r = \frac{2}{B\left(\frac{a+1}{a+2}, \frac{1}{2}\right)}. \tag{21}$$

Consequently the average concentration as a function of time becomes

$$\bar{m} = \left[ \bar{m}_Q^{-a} + \frac{a}{a+2} \frac{1}{2^{a+1}} \times B^{a+2}\left(\frac{a+1}{a+2}, \frac{1}{2}\right)(\tau - \tau_Q) \right]^{-1/a}. \tag{22}$$

The mass flux now follows from the mass balance

$$\frac{\mathrm{d}\bar{m}}{\mathrm{d}\tau} = -F X_i \tag{23}$$

with

$$F = -D_r X_i \left(\frac{\partial m}{\partial \phi}\right)_i \tag{24}$$

in which $X_i = \nu + 1$ and $F$ represents a flux parameter, which is related to the mass flux $n_{m,i}$ by

$$F = \frac{n_{m,i} R}{\rho_{m,o} D_o}. \tag{25}$$

For a slab ($\nu = 0$), the flux parameter $F$, according to equations (22) and (23) then becomes

$$F = \frac{1}{a+2} \frac{1}{2^{a+1}} B^{a+2}\left(\frac{a+1}{a+2}, \frac{1}{2}\right) \bar{m}^{a+1}. \tag{26}$$

Analytical solutions, similar to equations (22) and (26) are however not available for cylinder and sphere. Still, useful approximations can be constructed for these cases including the case of a slab as will be shown in the following equations.

Schoeber [10, 11] defined an average Sherwood number for the dispersed phase in the following way:

$$Sh_d = \frac{2F}{(\bar{m} - m_i)\bar{D}_r} \tag{27}$$

with

$$\bar{D}_r = \frac{1}{\bar{m} - m_i}\int_{m_i}^{\bar{m}} D_r \, \mathrm{d}m. \tag{28}$$

For $m_i = 0$ and $D_r = m^a$, equation (27) can be rewritten as

$$F = \frac{Sh_{d,a,v}}{2(a+1)}\bar{m}^{a+1}. \tag{29}$$

For $D_r = m^a$, $Sh_d$ is a function of $a$ and $v$ only and for the case of a slab, according to equations (26) and (29) can be expressed explicitly by

$$Sh_{d,a,0} = 4\left(\frac{a+1}{a+2}\right)\left[\frac{1}{2}B\left(\frac{a+1}{a+2}, \frac{1}{2}\right)\right]^{a+2}. \tag{30}$$

For cylinder and sphere, Schoeber determined $Sh_d$ numerically. Surprisingly, almost straight lines are obtained when $Sh_d$ values are plotted vs $a/(a+2)$ as is shown in Fig. 1, indicating an approximate linear relationship:

$$Sh_{d,a,v} = Sh_{d,0,v} + (Sh_{d,\infty,v} - Sh_{d,0,v})\left(\frac{a}{a+2}\right) \tag{31}$$

in which $Sh_{d,0,v}$ and $Sh_{d,\infty,v}$ represent the average Sherwood numbers for $a = 0$ and $a \to \infty$, respectively and are listed in Table 1.

Inserting these values in equation (31) then results in the following expressions:

$$Sh_{d,a,0} = \frac{\pi^2 + e^2 a}{a+2} \quad \text{(slab)} \tag{32}$$

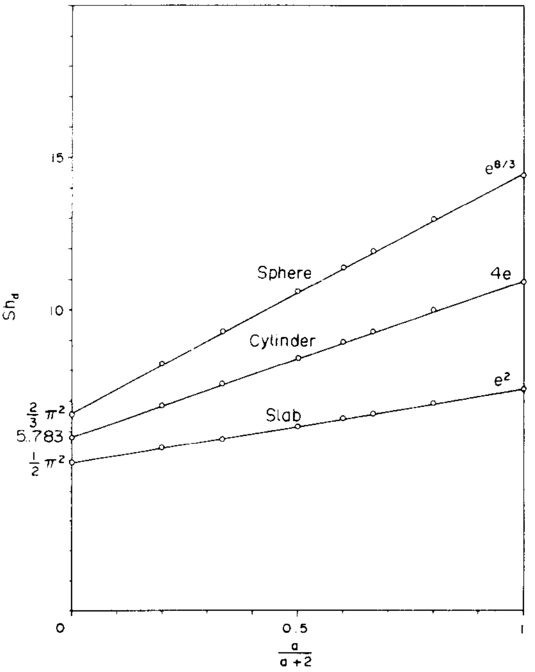

FIG. 1. The average Sherwood number for slab, cylinder and sphere and different values of $a$. (○) numerical, (—) linear approximation.

$$Sh_{d,a,1} = \frac{11.566 + 4\,\mathrm{e}a}{a+2} \quad \text{(cylinder)} \tag{33}$$

$$Sh_{d,a,2} = \frac{\frac{4}{3}\pi^2 + \mathrm{e}^{8/3}a}{a+2} \quad \text{(sphere).} \tag{34}$$

After substitution of equations (32)–(34) in equation (29), simple expressions for the flux parameter $F$ as a function of the power $a$ and the average concentration are obtained. It must however be realized that these approximate solutions do not cover the initial stage of the desorption process.

For this part of the process, an approximation, based on the short-time solution for a slab will be established later. First, two auxiliary variagles are introduced, i.e. the efficiency $E$ and the flux function $G$

$$E = 1 - \bar{m} \tag{35}$$

$$G = \frac{EF}{v+1}. \tag{36}$$

The particular solution for $F$, according to equation (29), expressed in terms of $E$ and $G$ then becomes

$$G = \frac{Sh_{d,a,v}}{2(a+1)(v+1)}E(1-E)^{a+1}. \tag{37}$$

For the derivatives with respect to $E$ of this flux function $G$ then follows:

$$G^{(1)} = \frac{1-(a+2)E}{E(1-E)}G \tag{38}$$

$$G^{(n)} = \frac{n-(a+2)E}{E(1-E)^n}(-1)^{n+1}\prod_{k=0}^{n-2}(a+1-k)G. \tag{39}$$

Obviously the flux function $G$ possesses a maximum $S$ for

$$E_S = \frac{1}{a+2} \tag{40}$$

and an inflection point $Q$ for

$$E_Q = \frac{2}{a+2} \tag{41}$$

which values follow from equations (38) and (39).

Once again it is stressed that this solution does not hold for the initial stage of the diffusion process. In order to establish that part of the solution, we must turn to the problem of determining the value of $G$ in the limit $E \to 0$. This value is equal for slab, cylinder and sphere, because the diffusion process at this stage takes place in an infinitesimally thin shell at the interface and

Table 1. The limit values of the average Sherwood numbers for slab, cylinder and sphere

| | Slab<br>$v = 0$ | Cylinder<br>$v = 1$ | Sphere<br>$v = 2$ |
|---|---|---|---|
| $Sh_{d,0,v}$ | $\frac{1}{2}\pi^2$ | 5.783 | $\frac{2}{3}\pi^2$ |
| $Sh_{d,\infty,v}$ | $\mathrm{e}^2$ | $4\,\mathrm{e}$ | $\mathrm{e}^{8/3}$ |

consequently the influence of curvature is still negligible.

$$\lim_{E\to 0} G_{a,0} = \lim_{E\to 0} G_{a,1} = \lim_{E\to 0} G_{a,2} = G_o. \quad (42)$$

For a constant diffusion coefficient ($a = 0$), $G_o$ can be found analytically from the short time solution for a slab [12]:

$$\bar{m} = m_o - 2(m_o - m_i)\left(\frac{\tau}{\pi}\right)^{1/2}. \quad (43)$$

Substitution in equation (35) gives

$$E = 2\left(\frac{\tau}{\pi}\right)^{1/2}. \quad (44)$$

While the flux parameter $F$ becomes

$$F = -\frac{\mathrm{d}\bar{m}}{\mathrm{d}\tau} = \frac{1}{\pi}\left(\frac{\tau}{\pi}\right)^{-1/2}. \quad (45)$$

Substitution in equation (36) then results in

$$G_o = \frac{2}{\pi}. \quad (46)$$

For values of $a > 0$, the limit value $G_o$ could not be determined analytically. However, the following relation appeared to be of sufficient accuracy:

$$G_o = G_{a,v,S} + \{G_{0,v,0} - G_{0,v,S}\}2^{-a} \quad (47)$$

in which $G_{0,v,0}$ represents $G_o$ for $a = 0$ and $G_{a,v,S}$ the particular solution of $G$ in point $S$, according to equation (37), which for $a = 0$ becomes

$$G_{0,v,S} = \frac{\pi^2}{16}. \quad (48)$$

Equation (47) then turns into

$$G_o = \frac{Sh_{d,a,0}}{2(a+1)(a+2)}\left(\frac{a+1}{a+2}\right)^{a+1} + \left(\frac{2}{\pi} - \frac{\pi^2}{16}\right)2^{-a} \quad (49)$$

in which $Sh_{d,a,0}$ follows from equation (32).

So far we have established solutions for short and large times. The problem that still remains, is how, starting from the "short time solution" $G_o$, the function $G$ goes over into the particular solution belonging to the regular regime. In order to solve this transition problem we have to define a transition point belonging to the regular regime. First we shall investigate the bounds of the regular regime. The regular regime possesses a lower bound due to the requirement that the centre concentration must always be lower than the initial centre concentration. In terms of the efficiency $E$, the use of the regular regime solution is therefore limited to the region $E \geqq E_T$. The efficiency in terms of the centre concentration $m_c$ reads

$$E = 1 - \bar{m} = 1 - \bar{g}_r m_c. \quad (50)$$

For the lower bound of the regular regime, corresponding to $m_c = 1$ then follows:

$$E_T = 1 - \bar{g}_r. \quad (51)$$

For a slab, $\bar{g}_r$ can be evaluated by applying equation (21). However, for cylinder and sphere, again no relations are available. A satisfactory approximation for values of $a > 0$ was found by plotting $\bar{g}_r^{-a}$ vs $a/(a + 2)$, which resulted in almost straight lines (Fig. 2), leading to the following relations for $\bar{g}_{r,a,v}$:

(a) Slab

$$\bar{g}_{r,a,0} = \left(\frac{a+2}{2 + \frac{1}{4}e^2 a}\right)^{1/a}$$

$$\text{for} \quad a > 0 \quad \text{and} \quad \bar{g}_{r,0,0} = \frac{2}{\pi}. \quad (52)$$

(b) Cylinder

$$\bar{g}_{r,a,1} = \left(\frac{a+2}{2 + ea}\right)^{1/a}$$

$$\text{for} \quad a > 0 \quad \text{and} \quad \bar{g}_{r,0,1} = 0.4318. \quad (53)$$

(c) Sphere

$$\bar{g}_{r,a,2} = \left(\frac{a+2}{2 + \frac{1}{4}e^{8/3} a}\right)^{1/a}$$

$$\text{for} \quad a > 0 \quad \text{and} \quad \bar{g}_{r,0,2} = \frac{3}{\pi^2}. \quad (54)$$

In Figs 3–5, $m_c$ is plotted vs $E$ for slab, cylinder and sphere and different values of $a$. In these diagrams also the locations of the inflection points $Q$ are indicated. It can easily be proved that $Q$ satisfies the condition $E_Q \geqq E_T$ for $v = 0, 1, 2$ and $a \geqq 0$, which means that point $Q$ stays within the bounds of the regular regime and can therefore be chosen as a transition point. As

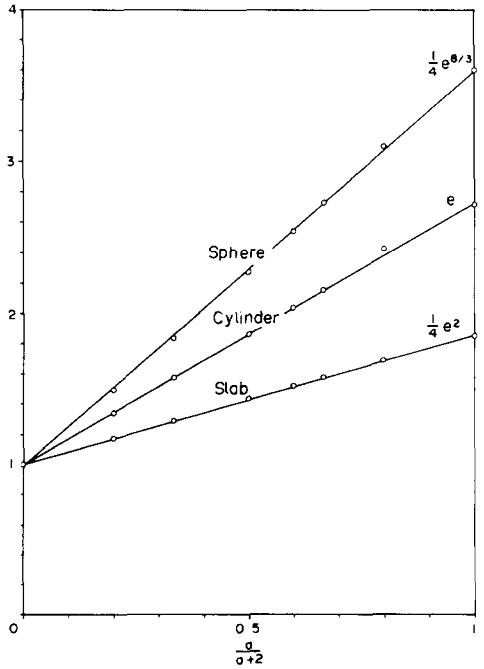

FIG. 2. The average reduced concentration for slab, cylinder and sphere and different values of $a$. (○) numerical, (—) linear approximation.

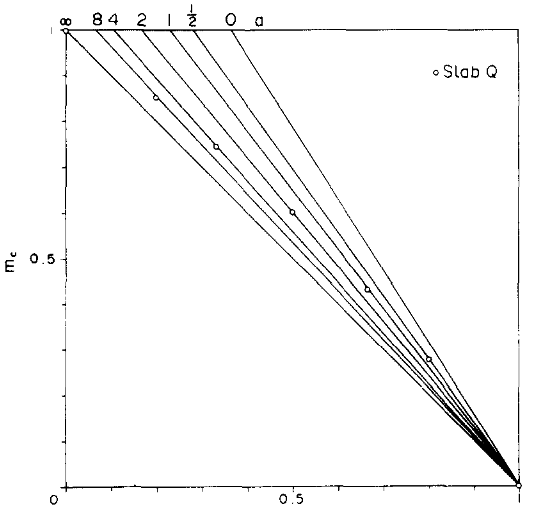

FIG. 3. Centre concentration $m_c$ in the regular regime vs the efficiency $E$ for a slab and different values of $a$.

follows from equation (41) the location of point $Q$ in the $E$ direction is independent of the geometry parameter $\nu$ and a function of $a$ only. For the transition region $0 < E \leqq E_Q$ the function $G$ is developed by means of a Taylor series expansion about the origin $0\{E = 0, G = G_o\}$:

$$G = G_o + EG_o^{(1)} + \frac{1}{2}E^2 G_o^{(2)} + \ldots \tag{55}$$

For a smooth transition in point $Q$ the Taylor series solution must at least satisfy the conditions: $G = G_Q$ and $G^{(1)} = G_Q^{(1)}$ in point $Q$. If these are the only conditions imposed on the transition, appropriate Taylor series approximations are:

(a) Slab

$$G = G_o + \frac{1}{5!}E^5 G_o^{(5)} + \frac{1}{6!}E^6 G_o^{(6)}. \tag{56}$$

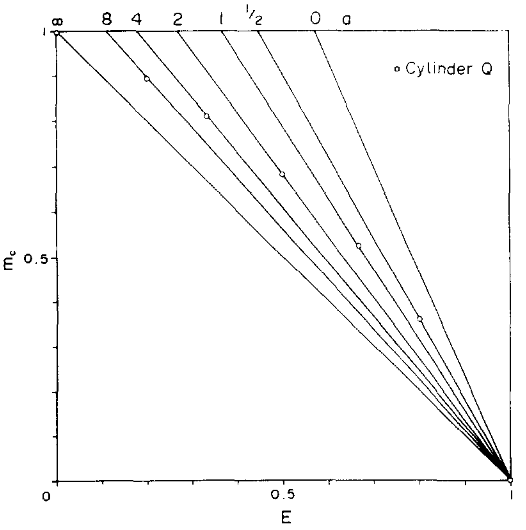

FIG. 4. Centre concentration $m_c$ in the regular regime vs the efficiency $E$ for a cylinder and different values of $a$.

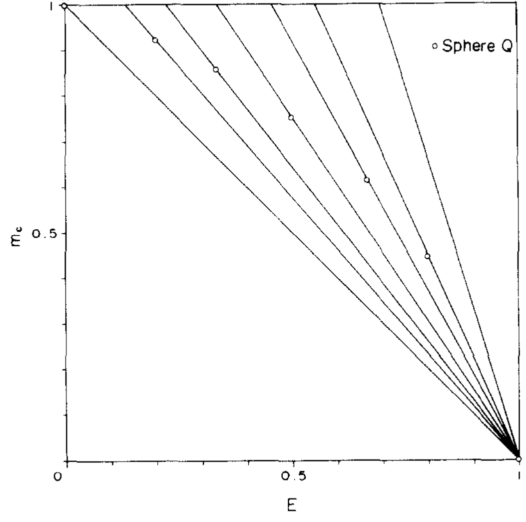

FIG. 5. Centre concentration $m_c$ in the regular regime vs the efficiency $E$ for a sphere and different values of $a$.

The two unknown derivatives $G_o^{(5)}$ and $G_o^{(6)}$ are evaluated with the aid of the two conditions in point $Q$, leading to

$$G_o^{(5)} = \frac{6!}{E_Q^5}\left\{G_Q - G_o - \frac{E_Q}{6}G_Q^{(1)}\right\} \tag{57}$$

$$G_o^{(6)} = \frac{5!}{E_Q^5}\left\{G_Q^{(1)} - \frac{1}{4!}E_Q^4 G_o^{(5)}\right\} \tag{58}$$

in which $G_Q$ and $G_Q^{(1)}$ follow from equations (37) and (38).

(b) Cylinder, sphere

$$G = G_o + EG_o^{(1)} + \frac{1}{2}E^2 G_o^{(2)} \tag{59}$$

with

$$G_o^{(1)} = \frac{2}{E_Q}\left\{G_Q - G_o + \frac{1}{2}E_Q G_Q^{(1)}\right\} \tag{60}$$

and

$$G_o^{(2)} = \frac{1}{E_Q}\{G_Q^{(1)} - G_o^{(1)}\}. \tag{61}$$

The flux in the transition region follows from equation (36) combined with equations (56) or (59). The desorption time follows from the mass balance

$$\frac{dE}{d\tau} = (\nu + 1)F. \tag{62}$$

Integration then leads to

$$\tau = \frac{1}{\nu + 1}\int_0^E \frac{1}{F}dE \quad \text{for} \quad 0 \leqq E \leqq E_Q \tag{63}$$

and

$$\tau = \tau_Q + \frac{1}{\nu + 1}\int_{E_Q}^E \frac{1}{F}dE \quad \text{for} \quad E > E_Q. \tag{64}$$

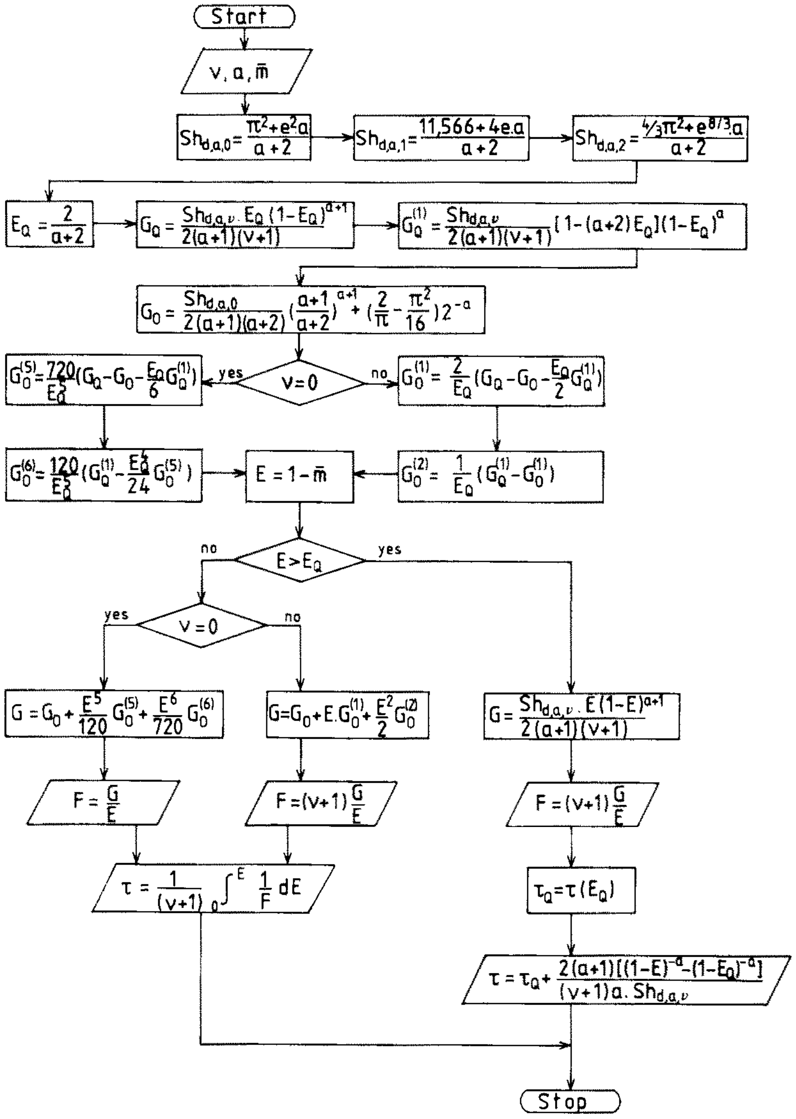

FIG. 6. Computational procedure for a desorption process in slabs and non-shrinking cylinders or spheres.

We shall first consider the interval $0 \leqq E \leqq E_Q$ and elaborate equation (63) for slab, cylinder and sphere by substitution of $F$.

(a) Slab

$$\tau = \int_0^E \frac{E}{G_o + \frac{E^5}{5!}G_o^{(5)} + \frac{E^6}{6!}G_o^{(6)}} \mathrm{d}E. \tag{65}$$

Unfortunately this integral cannot be transformed into a simple algebraic expression. However, a simple numerical evaluation using the trapezium rule already gives satisfactory results.

(b) Cylinder, sphere

$$\tau = \frac{1}{(v+1)^2}\int_0^E \frac{E}{G_o + EG_o^{(1)} + \frac{1}{2}E^2 G_o^{(2)}} \mathrm{d}E \tag{66}$$

$$= \frac{1}{(v+1)^2}\left[\frac{1}{G_o^{(2)}}\ln\left(\frac{G}{G_o}\right) - \frac{G_o^{(1)}}{G_o^{(2)}\sqrt{q}} \times \ln\left\{\frac{(G_o^{(2)}E + G_o^{(1)} - \sqrt{q})(G_o^{(1)} + \sqrt{q})}{(G_o^{(2)}E + G_o^{(1)} + \sqrt{q})(G_o^{(1)} - \sqrt{q})}\right\}\right]$$

with

$$q = \{G_o^{(1)}\}^2 - 2G_o G_o^{(2)}.$$

If $E = E_Q$ equations (65) and (66) can be used for the calculation of $\tau_Q$, the value of which must be known for the determination of the desorption time in the region $E > E_Q$. Substitution of $F$ according to equation (29) in equation (64) results in

$$\tau = \tau_Q + \frac{2(a+1)}{(v+1)a\,Sh_{d,a,v}} \times \{(1-E)^{-a} - (1-E_Q)^{-a}\}. \tag{67}$$

A complete outline for the computation of a desorption process in slabs and non-shrinking cylinders or non-shrinking spheres is given in Fig. 6.

### 3.2. *Shrinking systems*

When shrinkage of the system occurs during the desorption process, the mass flux has to be corrected for this phenomenon. Because the mass flux $j_{\mathrm{m,i}}$ in a reference component mass centered coordinate system is related to the flux parameter $F^*$ for shrinking systems by

$$F^* = \frac{j_{\mathrm{m,i}} d_{\mathrm{s},p} R_{\mathrm{s}}}{\rho_{\mathrm{m,o}} D_{\mathrm{o}} \rho_{\mathrm{s,o}}} \tag{68}$$

the correction for shrinkage can directly be applied to $F^*$. The mass balance for shrinking systems reads:

$$\frac{\mathrm{d}\bar{m}}{\mathrm{d}\tau} = -X_{\mathrm{i}}^* F^* \tag{69}$$

in which

$$X_{\mathrm{i}}^* = (\nu + 1)\left(1 + \frac{d_{\mathrm{s}}\rho_{\mathrm{m,o}}}{d_{\mathrm{m}}\rho_{\mathrm{s,o}}}\bar{m}\right)^{\nu/(\nu+1)} \tag{70}$$

and

$$F^* = -X_{\mathrm{i}}^* D_{\mathrm{r}}\left(\frac{\partial m}{\partial \phi}\right)_{\phi = 1}. \tag{71}$$

In the limit case $\tau \rightarrow 0$, for all values of $a \geqq 0$, the concentration profile approaches the rectangular shape of the initial profile, whereas the influence of shrinkage is still negligible implying the following relation:

$$\lim_{\tau \to 0} \frac{F^*}{X_{\mathrm{i}}^*} = \lim_{\tau \to 0} \frac{F}{X_{\mathrm{i}}} \tag{72}$$

or

$$\lim_{\tau \to 0} F^* = \lim_{\tau \to 0} \frac{X_{\mathrm{i}}^*}{X_{\mathrm{i}}} F = \left(1 + \frac{d_{\mathrm{s}}\rho_{\mathrm{m,o}}}{d_{\mathrm{m}}\rho_{\mathrm{s,o}}}\right)^{\nu/(\nu+1)} \lim_{\tau \to 0} F. \tag{73}$$

We define the shrinkage factor $H$ by

$$H = \frac{F^*}{F}. \tag{74}$$

From equation (73) then follows:

$$H_{\mathrm{o}} = \lim_{\tau \to 0} H = \left(1 + \frac{d_{\mathrm{s}}\rho_{\mathrm{m,o}}}{d_{\mathrm{m}}\rho_{\mathrm{s,o}}}\right)^{\nu/(\nu+1)}. \tag{75}$$

It was found by Schoeber that the correction for shrinkage in the regular regime can be described accurately by

$$H = 1 + \frac{\Delta Sh_{d,\nu}}{Sh_{d,a,\nu}} \quad \text{for} \quad E > E_Q \tag{76}$$

in which

$$\Delta Sh_{d,\nu} = Sh_{d,\infty,\nu}\left\{\left(1 + \frac{d_{\mathrm{s}}\rho_{\mathrm{m,o}}}{d_{\mathrm{m}}\rho_{\mathrm{s,o}}}\bar{m}\right)^{\nu/(\nu+1)} - 1\right\} \tag{77}$$

and $Sh_{d,a,\nu}$ representing the average Sherwood number for a non-shrinking system. The transition between the two limits of $H$ can be constructed by the following Taylor series expansion:

$$H = H_{\mathrm{o}} + \frac{E^2}{2} H_{\mathrm{o}}^{(0)} + \frac{E^3}{6} H_{\mathrm{o}}^{(3)} \quad \text{for} \quad 0 \leqq E \leqq E_Q \tag{78}$$

with

$$H_{\mathrm{o}}^{(2)} = \frac{6}{E_Q^2}\left\{H_Q - H_{\mathrm{o}} - \frac{E_Q}{3} H_Q^{(1)}\right\} \tag{79}$$

$$H_{\mathrm{o}}^{(3)} = \frac{2}{E_Q^2}\left\{H_Q^{(1)} - E_Q H_{\mathrm{o}}^{(2)}\right\}. \tag{80}$$

Finally, the shrinkage factor $H$ in the regular regime, expressed in terms of the efficiency $E$ becomes

$$H = 1 + \frac{Sh_{d,\infty,\nu}}{Sh_{d,a,\nu}}\left[\left\{1 + \frac{d_{\mathrm{s}}\rho_{\mathrm{m,o}}}{d_{\mathrm{m}}\rho_{\mathrm{s,o}}}(1 - E)\right\}^{\nu/(\nu+1)} - 1\right] \quad \text{for} \quad E > E_Q. \tag{81}$$

The determination of the desorption time now offers no more problems. Integration of the mass balance leads to

$$\tau = \frac{1}{(\nu+1)}\int_0^E \left[F^*\left\{1 + \frac{\mathrm{d}_{\mathrm{s}}\rho_{\mathrm{m,o}}}{d_{\mathrm{m}}\rho_{\mathrm{s,o}}}(1-E)\right\}^{\nu/(\nu+1)}\right]^{-1} \mathrm{d}E \quad \text{for} \quad 0 \leqq E \leqq E_Q \tag{82}$$

and

$$\tau = \tau_Q + \frac{1}{(\nu+1)}\int_{E_Q}^E \left[F^*\left\{1 + \frac{d_{\mathrm{s}}\rho_{\mathrm{m,o}}}{d_{\mathrm{m}}\rho_{\mathrm{s,o}}}(1-E)\right\}^{\nu/(\nu+1)}\right]^{-1} \mathrm{d}E \quad \text{for} \quad E > E_Q. \tag{83}$$

In Fig. 7 the computational procedure for shrinking systems is presented.

## 4. A COMPARISON BETWEEN THE RESULTS OBTAINED WITH THE APPROXIMATE METHOD AND OBTAINED NUMERICALLY

The exact solution was obtained by solving the diffusion equation numerically, using finite differences and the Crank–Nicolson implicit method with variable implicitness [10, 11].

The approximate solution was obtained by straightforward calculations, following the computation procedures as indicated in Figs. 6 and 7. In Figs 8–10 the flux function $G$ is plotted vs the efficiency $E$ for slab, cylinder and sphere and for different values of $a$. As can be seen, hardly any differences occur between the exact (numerical) and approximate solutions. The same conclusion can be drawn for a shrinking sphere (Fig. 11), for which also the desorption time was calculated as a function of the efficiency $E$ by the approximate method and compared with the exact solution (Fig. 12).

Eventually an improvement in computational speed of a factor 1000 was observed by applying the approximate method instead of the numerical method mentioned above.

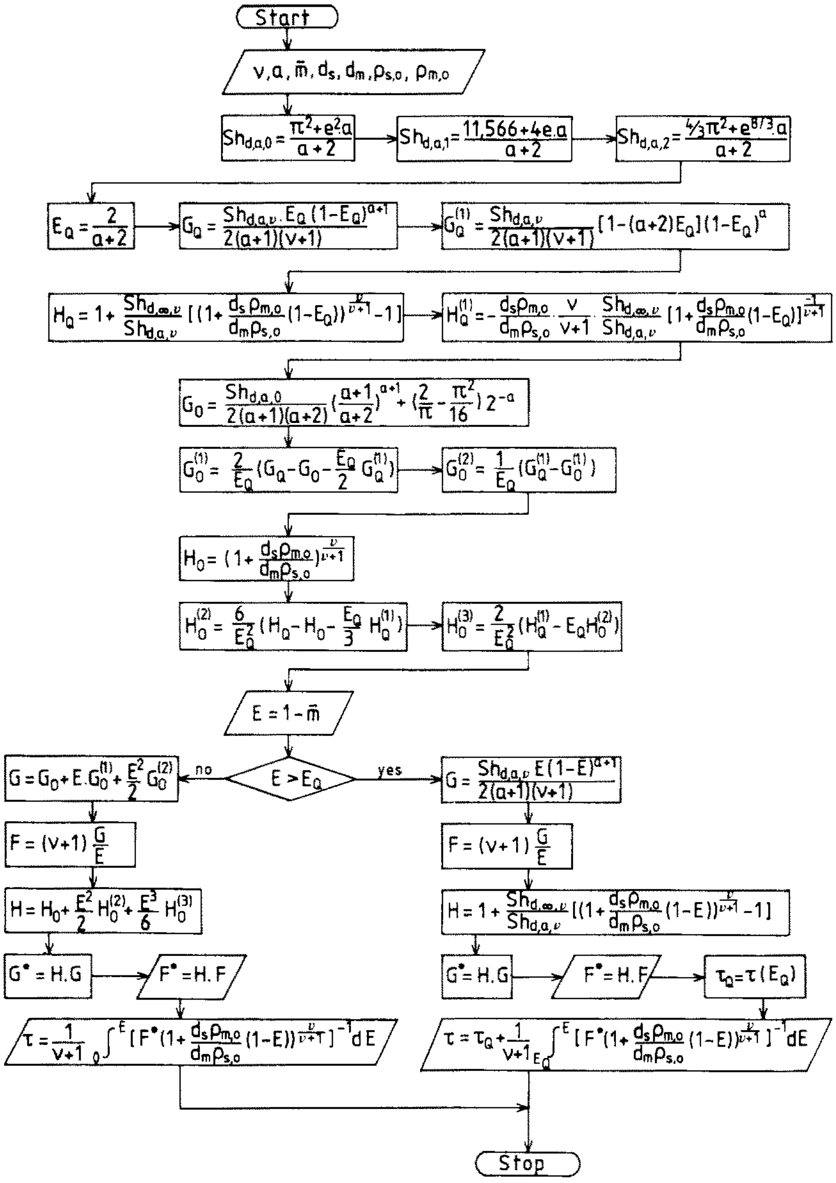

FIG. 7. Computational procedure for a desorption process in shrinking cylinders or spheres.

From these observations we may conclude that the approximate method developed here gives accurate results, the computational effort for the determination of the desorption time being reduced to pocket calculator level.

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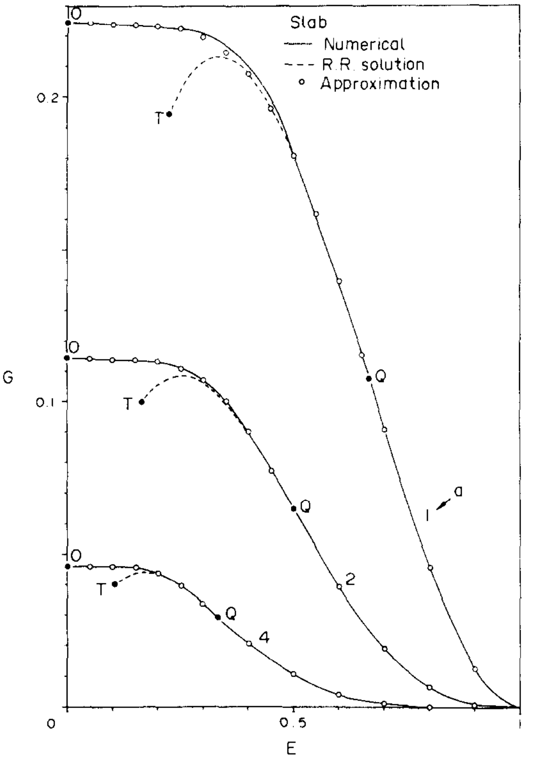

FIG. 8. The function $G$ (see text) vs the efficiency $E$ for a slab.

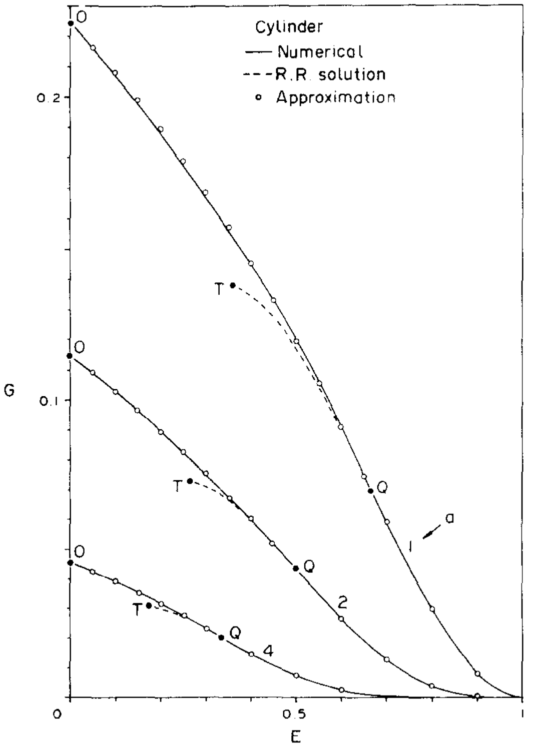

FIG. 9. The function $G$ vs the efficiency $E$ for a cylinder.

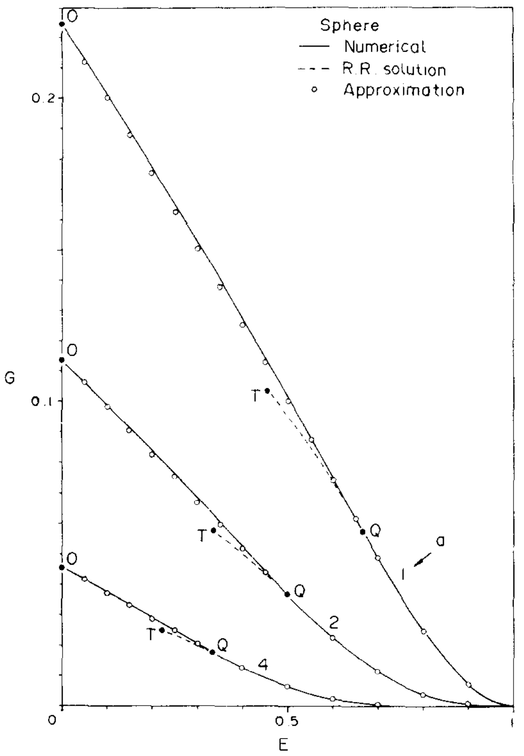

FIG. 10. The function $G$ vs the efficiency $E$ for a sphere.

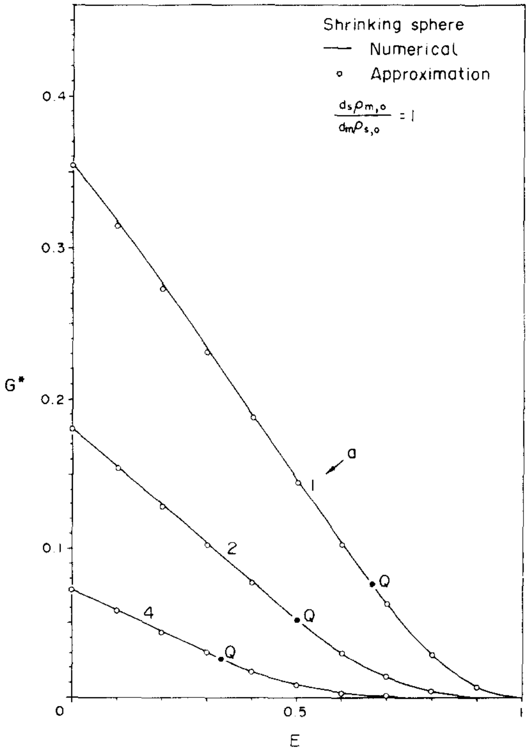

FIG. 11. The function $G^*$ vs the efficiency $E$ for a shrinking sphere.

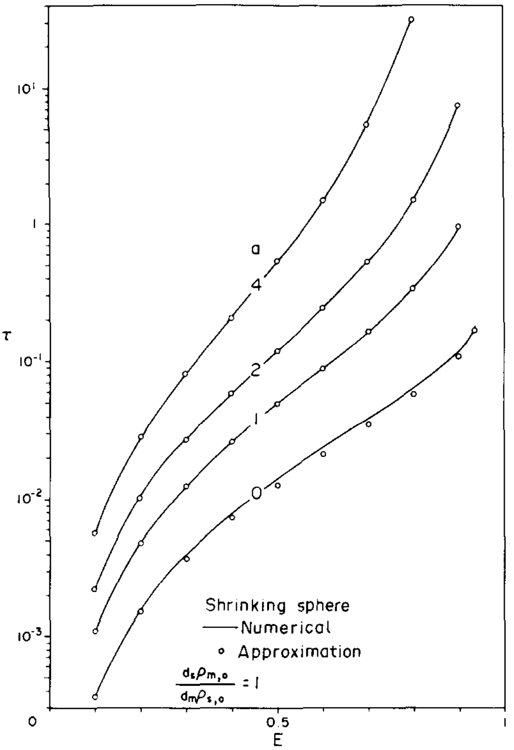

FIG. 12. The desorption time $\tau$ vs the efficiency $E$ for a shrinking sphere.

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## APPENDIX A

*Derivation of the average value of* $g_r$

The average value of $g_r$ is determined by

$$g_r = \int_0^1 g_r \, \mathrm{d}\phi \tag{A1}$$

with at $\phi = 0$, $g_r = 1$ and at $\phi = 1$, $g_r = 0$.
Integration by parts of equation (A1) then leads to

$$\bar{g}_r = \int_0^1 \phi \, \mathrm{d}g_r \tag{A2}$$

with according to equation (18):

$$\phi = 1 - \frac{B_z\left(\dfrac{a+1}{a+2}, \dfrac{1}{2}\right)}{B\left(\dfrac{a+1}{a+2}, \dfrac{1}{2}\right)}. \tag{A3}$$

Evaluation of the right hand integral in equation (A2) finally results in

$$\bar{g}_r = \frac{2}{B\left(\dfrac{a+1}{a+2}, \dfrac{1}{2}\right)}. \tag{A4}$$

## UNE METHODE APPROCHEE DE RESOLUTION DU PROBLEME DE DIFFUSION NON LINEAIRE AVEC UNE LOI PUISSANCE ENTRE LE COEFFICIENT DE DIFFUSION ET LA CONCENTRATION—I. CALCUL DES TEMPS DE DESORPTION

**Résumé**—On propose une méthode pour le calcul approché de la concentration qui dépend de la diffusion par une loi puissance ($D_r = m^a$). Cette méthode peut être appliquée au mécanisme de désorption dans des systemes qui se contractent ou non, avec, une géométrie plane, cylindrique ou sphérique. La méthode est développée pour une désorption partant d'un profil de concentration uniforme et des conditions de Dirichlet, c'est-à-dire concentration uniforme à la surface et symétrique par rapport au centre, à l'axe ou au plan médian du système. La méthode peut être utilisée pour prévoir l'évolution au cours du temps de la concentration et du flux, avec l'approximation des solutions exactes, obtenues par des techniques analytiques ou numériques.

## EINE NÄHERUNGSMETHODE ZUR LÖSUNG DES NICHTLINEAREN DIFFUSIONSPROBLEMS MIT EINER POTENZBEZIEHUNG ZWISCHEN DIFFUSIONSKOEFFIZIENT UND KONZENTRATION—I. BERECHNUNG VON DESORPTIONSZEITEN

**Zusammenfassung**—Es wird eine Methode für die näherungsweise Berechnung der konzentrationsabhängigen Diffusion mit einer Potenzbeziehung zwischen Diffusionskoeffizient und Konzentration (von der Form $D_r = m^a$) vorgeschlagen. Diese Methode kann auf den Desorptionsvorgang in nicht-schrumpfenden oder schrumpfenden Systemen mit Platten-, Zylinder- oder Kugelgeometrie angewandt werden und wird entwickelt für die Desorption bei anfänglich gleichförmigem Konzentrationsprofil und Dirichlet-Randbedingungen d.h. konstante Oberflächenkonzentration und Symmetrie in bezug auf das Zentrum, die Mittellinie bzw. die Mittelebene des Systems. Schließlich kann die Methode verwendet werden, um das Zeitverhalten von mittlerer Konzentration und mittlerem Diffusionsstrom zu berechnen, was zu recht genauen Approximationen der exakten Lösung, die man analytisch oder numerisch erhält, führt.

# ПРИБЛИЖЕННЫЙ МЕТОД РЕШЕНИЯ ЗАДАЧИ НЕЛИНЕЙНОЙ ДИФФУЗИИ ПРИ СТЕПЕННОЙ ЗАВИСИМОСТИ КОЭФФИЦИЕНТА ДИФФУЗИИ ОТ КОНЦЕНТРАЦИИ.

## I. РАСЧЕТ ВРЕМЕНИ ДЕСОРБЦИИ

**Аннотация** — Предложен метод приближенного расчета концентрации в задаче диффузии при степенной зависимости коэффициента диффузии от концентрации ($D_r = m^a$), который может быть использован для описания процесса десорбции в системах с усадкой и без, имеющих форму пластины, цилиндра или шара. Метод разработан для процесса десорбции при однородном начальном профиле концентрации и условиями Дирихле на границе, т. е. постоянной концентрации вещества на поверхности и условиями симметрии по отношению к центру, центральной оси или центральной плоскости системы. В конечном счете, его можно использовать для расчета временной зависимости средней концентрации и величины потока, причем результаты хорошо согласуются с аналитическими и численными решениями.