

AN APPROXIMATE METHOD FOR THE NONLINEAR DIFFUSION PROBLEM WITH A POWER RELATION BETWEEN DIFFUSION COEFFICIENT AND CONCENTRATION—II. COMPUTATION OF CONCENTRATION PROFILES

J. K. LIOU and S. BRUIN

Department of Process Engineering, Agricultural University Wageningen,
 De Dreijen 12, 6703 BC Wageningen, The Netherlands

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Abstract—The approximate method, developed in part I [*Int. J. Heat Mass Transfer* **25**, 1209–1220 (1982)] is extended with approximate relations for the computation of concentration profiles in a nonlinear desorption process with Dirichlet boundary conditions and a power-function variation of the diffusion coefficient with concentration. The relations are applicable to non-shrinking or shrinking systems with slab, cylindrical or spherical geometry.

NOMENCLATURE

a ,	power in concentration dependence of the diffusion coefficient;
b ,	parameter, occurring in equation (41);
B, B_z ,	beta function, incomplete beta function;
D ,	diffusion coefficient [$\text{m}^2 \text{s}^{-1}$];
E ,	efficiency desorption process;
f ,	time dependent part of the large time solution;
g ,	space dependent part of the large time solution;
J_0, J_1 ,	Bessel functions of zero and first order;
$K_{1/4}$,	modified Bessel function of order 1/4;
m ,	dimensionless concentration;
P ,	parameter in equations (4), (5) and (9);
Sh_d ,	average Sherwood number of the dispersed phase;
y ,	variable defined in equation (18);
z ,	auxiliary variable (app. A, B).

Greek symbols

λ ,	separation parameter in equation (3);
μ_n ,	n th eigenvalue;
ν ,	geometry parameter;
ϕ ,	dimensionless space coordinate;
τ ,	dimensionless time.

Subscripts

c ,	centre;
Q ,	referring to transition point Q (part I);
R ,	referring to upper bound of transition region;
T ,	referring to lower bound of transition region.

Superscripts

$\bar{}$,	average value;
$*$,	referring to shrinking systems;

$'$,	referring to the short time solution;
$''$,	referring to the large time solution.

1. INTRODUCTION

AS WAS discussed in part I [1], only the particular solution for large times of the diffusion equation for a slab can be expressed in terms of known analytical functions. This solution, however, is rather cumbersome to handle due to its implicit form and the necessary evaluations of the beta functions involved. Furthermore this solution does not include the initial stage of the desorption process and is only valid for the case of slab geometry, whereas the problem for cylinder and sphere remains unsolved.

In this paper our major concern will therefore be the construction of approximate relations for the computation of concentration profiles in slab, cylinder and sphere. By combining existing analytical solutions for the limiting cases, $a = 0$ (constant diffusion coefficient) and $a \rightarrow \infty$, satisfactory approximations were obtained for the general case of nonlinear diffusion with a concentration dependent diffusion coefficient of the type $D_c = m^a$. Although the composite approximations have no rigorous analytical background, they appear to be quite useful for computational purposes, due to their simplicity and accuracy, and for that reason are a feasible alternative to the numerical solution, in particular for engineering applications.

In section 2 we will treat the approximations for large and short times respectively. In addition an appropriate transition criterion is formulated in order to link both limiting approximations. In section 3 we will compare the concentration profiles, obtained by employing the approximate relations and by solving the diffusion equation numerically. The numerical evaluation of concentration profiles was achieved by applying a finite difference technique, following the

Crank–Nicolson method with variable implicitness [2–4] for discretization. Moreover, another technique, involving orthogonal collocation, was employed for obtaining the large time solution [5].

As we will frequently refer to equations or figures from part I, the reader is suggested to consult part I as much as possible.

2. APPROXIMATE RELATIONS FOR CONCENTRATION PROFILES

2.1. The large time solution

In this section our attention will be focussed on the particular solution of the diffusion equation for large times. As was mentioned in our previous paper [1], separation of variables in the diffusion equation leads only to a solution for the case of a slab. However, as will be shown in the following, satisfactory approximations, based on known analytical solutions for the special cases, $a = 0$ (constant diffusion coefficient) and $a \rightarrow \infty$, can be constructed for slab, cylinder and sphere. For non-shrinking systems with $D_r = m^a$, the diffusion equation, according to equation (1) of part I becomes

$$\frac{\partial m}{\partial \tau} = \frac{\partial}{\partial \phi} \left(m^a (v+1)^2 \phi^{2v/(v+1)} \frac{\partial m}{\partial \phi} \right). \quad (1)$$

Separation of variables is achieved by substituting $m(\phi, \tau) = f(\tau)g(\phi)$ in equation (1), resulting in two ordinary differential equations

$$\frac{1}{f^{a+1}} \frac{df}{d\tau} = \lambda \quad (2)$$

and

$$\frac{1}{g} \frac{d}{d\phi} \left(g^a (v+1)^2 \phi^{2v/(v+1)} \frac{dg}{d\phi} \right) = \lambda. \quad (3)$$

In terms of the reduced variable $g_r = g/g_c$, equation (3) becomes

$$\frac{d}{d\phi} \left(g_r^a \phi^{2v/(v+1)} \frac{dg_r}{d\phi} \right) = -P_{a,v} g_r \quad (4)$$

with

$$P_{a,v} = \frac{-\lambda}{(v+1)^2 g_c^a}. \quad (5)$$

Substitution of $\bar{m} = f\bar{g}$ in equation (2) yields

$$\lambda = \frac{1}{f^a \bar{m}} \frac{d\bar{m}}{d\tau}. \quad (6)$$

According to equations (23) and (29) of part I the mass balance is expressed by

$$\frac{d\bar{m}}{d\tau} = \frac{-(v+1)Sh_{d,a,v}}{2(a+1)} \bar{m}^{a+1}. \quad (7)$$

Substitution of equation (7) in equation (6) then gives

$$\lambda = \frac{-(v+1)Sh_{d,a,v}}{2(a+1)f^a} \bar{m}^a = \frac{-(v+1)Sh_{d,a,v}}{2(a+1)} \bar{g}^a \quad (8)$$

whereas substitution of equation (8) in equation (5) gives

$$P_{a,v} = \frac{Sh_{d,a,v} \bar{g}_r^a}{2(v+1)(a+1)}. \quad (9)$$

If we assume the large time solution to be valid in point $Q(\tau_Q, \bar{m}_Q)$ as defined in part I, integration of equation (7) results in

$$\bar{m} = \left[\bar{m}_Q^{-a} + \frac{(v+1)aSh_{d,a,v}}{2(a+1)} (\tau - \tau_Q) \right]^{-1/a}. \quad (10)$$

Furthermore we may express the particular solution as

$$m(\phi, \tau) = \frac{g_r(\phi)}{\bar{g}_r} \bar{m} \quad (11)$$

leading to

$$m(\phi, \tau) = \frac{g_r(\phi)}{\bar{g}_r} \left[\bar{m}_Q^{-a} + \frac{(v+1)aSh_{d,a,v}}{2(a+1)} (\tau - \tau_Q) \right]^{-1/a}. \quad (12)$$

As an alternative we may express this solution in terms of the efficiency E , rather than in terms of the time variable τ , yielding

$$m(\phi, E) = \frac{g_r(\phi)}{\bar{g}_r} (1 - E) \quad (13)$$

where $g_r(\phi)$ and \bar{g}_r follow from equation (4), which is subject to the boundary conditions

$$\phi^{v/(v+1)} \frac{dg_r}{d\phi} = 0 \quad \text{and} \quad g_r = 1 \quad \text{at} \quad \phi = 0 \quad (14)$$

$$g_r = 0 \quad \text{at} \quad \phi = 1. \quad (15)$$

This nonlinear differential equation can be classified as a specific case of the Emden–Fowler equation, discussed extensively by Fowler [6] in relation to astrophysics and more recently has found a renewed interest in the context of diffusion with chemical reaction [7]. An analytical solution for the case of a slab ($v = 0$) is derived in appendix A, leading to the implicit relation, already given in part I. For the average value of g_r , we derived

$$\bar{g}_r = \frac{2}{B\left(\frac{a+1}{a+2}, \frac{1}{2}\right)} \quad (16)$$

whereas, from equations (9) and (16) and (A7) we find

$$Sh_{d,a,0} = \left(\frac{a+1}{a+2}\right) 2^{-a} B^{a+2} \left(\frac{a+1}{a+2}, \frac{1}{2}\right) \quad (17)$$

Substitution of these analytical results in equations (12) or (13) results in the concentration profile as a function of either time τ or efficiency E . This solution, however, still contains the function $g_r(\phi)$ which cannot be evaluated directly from its inverse function $\phi(g_r)$.

In order to examine the possibility of constructing approximate relations for the still unsolved cases of

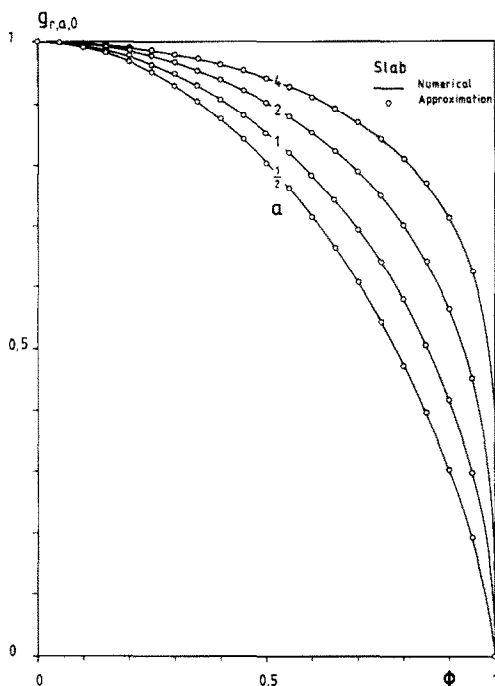


FIG. 1. The reduced concentration profile $g_{r,a,0}$ for a slab at different values of a . (—): numerical, (○): approximation by equation (25).

cylinder and sphere, a numerical solution of equation (4) was produced by an orthogonal collocation method [5]. An analysis of the numerical solution showed that the concentration profile is approximated by the simple relation

$$y_{a,v} = y_{0,v} + (y_{\infty,v} - y_{0,v}) \left(\frac{a}{a+1} \right) \quad \text{with } y_{a,v} = g_{r,a,v}^{a+1} \quad (18)$$

Since the limiting solutions $y_{0,v}$ and $y_{\infty,v}$ are known analytical functions, the evaluation of $g_{r,a,v}$ from equation (18) becomes an easy task. Figures 1, 2 and 3 show the approximations for $g_{r,a,v}$ together with the numerical solution of equation (4) by the orthogonal collocation method mentioned above.

For a constant diffusion coefficient ($a = 0$) the analytical solutions are obtained from the first eigenfunctions of the well known series solutions for slab, cylinder and sphere [8]

$$y_{0,0} = g_{r,0,0} = \cos\left(\frac{1}{2}\pi\phi\right) \quad (\text{slab}) \quad (19)$$

$$y_{0,1} = g_{r,0,1} = J_0(\mu_1\phi^{1/2}) \quad (\text{cylinder}) \quad (20)$$

in which $\mu_1 = 2.40483$ is the first positive root of $J_0(\mu_n) = 0$, with J_0 representing the zero order Bessel function (in appendix B a polynomial approximation of the Bessel function $J_0(\mu_1\phi^{1/2})$ is given for computational purposes [9]),

$$y_{0,2} = g_{r,0,2} = \frac{\sin(\pi\phi^{1/3})}{\pi\phi^{1/3}} \quad (\text{sphere}). \quad (21)$$

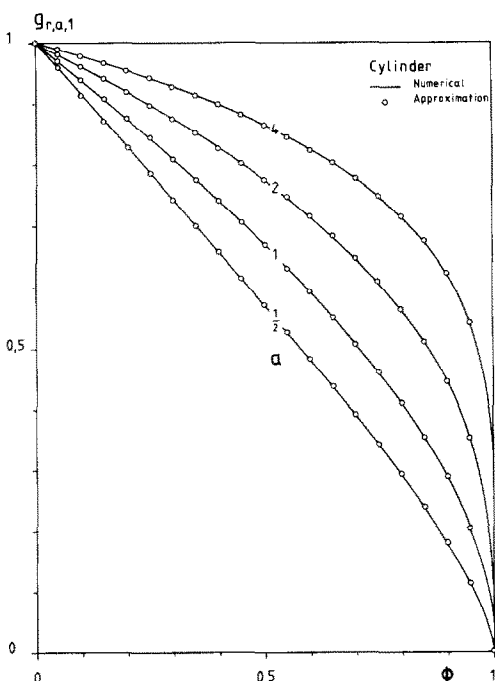


FIG. 2. The reduced concentration profile $g_{r,a,1}$ for a cylinder at different values of a . (—): numerical, (○): approximation by equation (26).

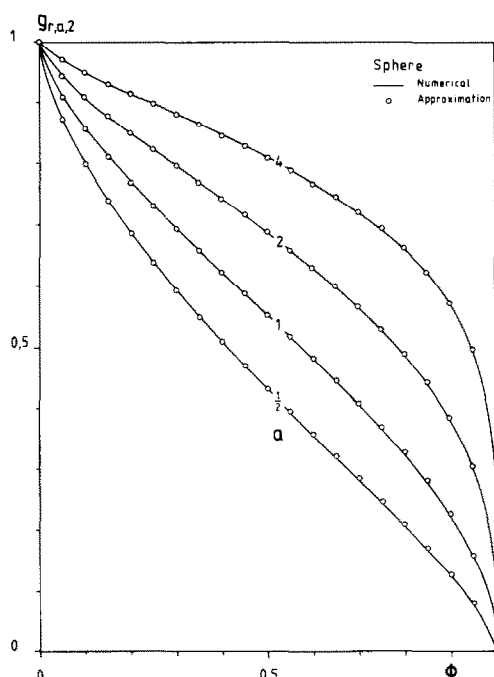


FIG. 3. The reduced concentration profile $g_{r,a,2}$ for a sphere at different values of a . (—): numerical, (○): approximation by equation (27).

If equation (4) is expressed in terms of y

$$\frac{d}{d\phi} \left(\phi^{2v/(v+1)} \frac{dy}{d\phi} \right) = -P_{\infty, v}(a+1)y^{1/(a+1)} \quad (22)$$

the limiting form of this equation for $a \rightarrow \infty$ becomes

$$\frac{d}{d\phi} \left(\phi^{2v/(v+1)} \frac{dy}{d\phi} \right) = -P_{\infty, v}(a+1). \quad (23)$$

Equation (23) was solved by Schroeber [2], resulting in

$$y_{\infty, v} = 1 - \phi^{2/(v+1)}. \quad (24)$$

After substitution of the limiting solutions in equation (18), the following relations are obtained:

$$g_{r, a, 0} = \left\{ \cos\left(\frac{1}{2}\pi\phi\right) + \left[1 - \phi^2 - \cos\left(\frac{1}{2}\pi\phi\right)\right] \times \left(\frac{a}{a+1}\right) \right\}^{1/(a+1)}, \quad (\text{slab}) \quad (25)$$

$$g_{r, a, 1} = \left\{ J_0(\mu_1\phi^{1/2}) + [1 - \phi - J_0(\mu_1\phi^{1/2})] \times \left(\frac{a}{a+1}\right) \right\}^{1/(a+1)}, \quad (\text{cylinder}) \quad (26)$$

$$g_{r, a, 2} = \left\{ \frac{\sin(\pi\phi^{1/3})}{\pi\phi^{1/3}} + \left[1 - \phi^{2/3} - \frac{\sin(\pi\phi^{1/3})}{\pi\phi^{1/3}}\right] \times \left(\frac{a}{a+1}\right) \right\}^{1/(a+1)}. \quad (\text{sphere}) \quad (27)$$

Together with the approximate relations (52), (53) and (54) from part I for the average values of $g_{r, a, v}$ substitution in equation (13) finally results in the following expressions for the concentration $m_{a, v}$:

2.1.1. Slab.

$$m_{0, 0} = \frac{\pi}{2} \cos\left(\frac{1}{2}\pi\phi\right)(1-E) \quad (a=0) \quad (28)$$

and

$$m_{a, 0} = \left(\frac{2 + \frac{1}{4}e^2a}{a+2}\right)^{1/a} \left[\frac{\cos(\frac{1}{2}\pi\phi)}{a+1} + \frac{a(1-\phi^2)}{a+1} \right]^{1/(a+1)} (1-E). \quad (a>0) \quad (29)$$

2.1.2. Cylinder.

$$m_{0, 1} = \frac{\mu_1}{2J_1(\mu_1)} J_0(\mu_1\phi^{1/2})(1-E) \quad (a=0) \quad (30)$$

and

$$m_{a, 1} = \left(\frac{2+ea}{a+2}\right)^{1/a} \left[\frac{J_0(\mu_1\phi^{1/2})}{a+1} + \frac{a(1-\phi)}{a+1} \right]^{1/(a+1)} (1-E) \quad (a>0) \quad (31)$$

in which $J_1(\mu_1) = 0.51915$ with J_1 the Bessel function of order 1.

2.1.3. Sphere.

$$m_{0, 2} = \frac{\pi^2}{3} \frac{\sin(\pi\phi^{1/3})}{\pi\phi^{1/3}} (1-E) \quad (a=0) \quad (32)$$

and at $\phi=0$

$$m_{c, 0, 2} = \frac{\pi^2}{3} (1-E) \quad (33)$$

whereas,

$$m_{a, 2} = \left(\frac{2 + \frac{1}{4}e^{8/3}a}{a+2}\right)^{1/a} \left[\frac{\sin(\pi\phi^{1/3})}{(a+1)(\pi\phi^{1/3})} + \frac{a(1-\phi^{2/3})}{a+1} \right]^{1/(a+1)} (1-E) \quad (a>0) \quad (34)$$

and at $\phi=0$

$$m_{c, a, 2} = \left(\frac{2 + \frac{1}{4}e^{8/3}a}{a+2}\right)^{1/a} (1-E) \quad (35)$$

These approximations give explicitly the concentration profiles for large times. The efficiency E is related to the time variable τ (desorption time) by equation (67) of part I. For short times however, application of the relations given above leads to erroneous results, but as will be shown in the following section, simple approximations can also be constructed for the initial stage of the diffusion process.

2.2. The short time solution

For a constant diffusion coefficient, the short time solutions for slab, cylinder and sphere can be expressed by the first order approximation of an error function series [8]:

2.2.1. Slab.

$$m_{0, 0} = 1 - \operatorname{erfc}\left(\frac{1-\phi}{2\tau^{1/2}}\right) - \operatorname{erfc}\left(\frac{1+\phi}{2\tau^{1/2}}\right) \quad (36)$$

2.2.2. Cylinder.

$$m_{0, 1} = 1 - \phi^{-1/4} \operatorname{erfc}\left(\frac{1-\phi^{1/2}}{2\tau^{1/2}}\right) \quad (37)$$

with, at $\phi=0$

$$m_{c, 0, 1} = 1 - \frac{e^{-1/8\tau}}{(\pi\tau)^{1/2}} K_{1/4}(1/8\tau). \quad (38)$$

in which $K_{1/4}$ represents the modified Bessel function of order $\frac{1}{4}$. A computational formula of this function for large values of the argument is given in appendix B.

2.2.3. Sphere.

$$m_{0, 2} = 1 - \phi^{-1/3} \times \left[\operatorname{erfc}\left(\frac{1-\phi^{1/3}}{2\tau^{1/2}}\right) - \operatorname{erfc}\left(\frac{1+\phi^{1/3}}{2\tau^{1/2}}\right) \right] \quad (39)$$

with, at $\phi=0$

$$m_{c, 0, 2} = 1 - \frac{2}{(\pi\tau)^{1/2}} e^{-1/4\tau}. \quad (40)$$

For nonzero values of the power a , Friedmann [10] solved the diffusion equation for a semi-infinite slab. His second order approximation is however only applicable in case of small fractional values of a , either positive or negative. As we are not only interested in weak dependences, another approach is necessary in order to arrive at less restrictive relations which in addition cover the cases of cylinder and sphere as well. At this point it is desirable to leave the path of exact analytical solutions and turn our attention to feasible approximations. A particularly simple relation appeared to be of substantial value in approximating the initial stage of the diffusion process

$$m_{a,v} = (m_{0,v})^b$$

$$\text{with } b = \frac{1}{(a+1)} - \frac{a(v+1)}{2(v+2)(a+1)(a+2)} \quad (41)$$

in which $m_{0,v}$ represents the short time solution for a constant diffusion coefficient ($a = 0$), and is expressed by equations (36)–(40). As long as the centre concentration does not alter excessively, equation (41) provides a satisfactory approximation.

2.3. The transition region

In order to effectuate a gradual transition between the short time and large time approximations, a region is defined, in which a complete transition from the short time to the large time concentration profile is

established. In part I we examined the bounds of the regular regime, resulting in a lower bound T , for which

$$E_T = 1 - \bar{g}_{r,a,v} \quad (42)$$

For $E < E_T$, the large time approximation becomes impossible, because the centre concentration exceeds unity. As for the upper bound of the transition region, point Q (part I), was already defined as a transition point belonging to the regular regime. The concentration profile, however, will exhibit much resemblance to the regular regime profile, long before point Q is reached. In examining the flux function G for a slab (part I), we observe that in point S , corresponding to the occurring maximum in the regular regime solution for G , the difference between the G curve and the regular regime solution has already become very small. Consequently, the concentration profile in point S is expected not to differ very much from the regular profile, indicating that point S may also serve as an upper bound of the transition region. Unfortunately, for cylinder and sphere, the maximum in the regular regime solution for G is located in the region $E < E_T$ and therefore is useless as an upper bound. For that reason we define the upper bound of the transition region for cylinder and sphere as the value of E at which the centre concentration is equal to the centre concentration in point S for a slab.

According to equations (40) and (50) of part I, the

Table 1. Approximate relations for the computation of concentration profiles in case of a concentration dependent diffusion coefficient of the type: $D_r = m^a$

SLAB ($v=0$)	CYLINDER ($v=1$)	SPHERE ($v=2$)
Short time approximations with: $b = \frac{1}{a+1} - \frac{a(v+1)}{2(v+2)(a+1)(a+2)}$ (penetration period: $E < E_T$)		
$m'_{a,0} = [1 - \operatorname{erfc}(\frac{1-\Phi}{2\sqrt{\tau}}) - \operatorname{erfc}(\frac{1+\Phi}{2\sqrt{\tau}})]^b$	$m'_{a,1} = [1 - \Phi^{-1/4} \operatorname{erfc}(\frac{1-\Phi^{1/2}}{2\sqrt{\tau}})]^b$ $m'_{c,a,1} = [1 - (\pi\tau)^{-1/2} e^{-1/8\tau} K_{1/4}(\frac{1}{8\tau})]^b$	$m'_{a,2} = [1 - \Phi^{-1/3} (\operatorname{erfc}(\frac{1-\Phi^{1/3}}{2\sqrt{\tau}}) - \operatorname{erfc}(\frac{1+\Phi^{1/3}}{2\sqrt{\tau}}))]^b$ $m'_{c,a,2} = [1 - 2(\pi\tau)^{-1/2} e^{-1/4\tau}]^b$
Large time approximations (regular regime: $E > E_R$)		
$m''_{0,0} = \frac{\pi}{2} \cos(\frac{1}{2}\pi\Phi)[1-E]$ $m''_{a,0} = (\frac{2+\frac{1}{2}e^2a^{1/a}}{a+2}) [\frac{\cos(\frac{1}{2}\pi\Phi)}{a+1} + \frac{a(1-\Phi^2)^{\frac{1}{a+1}}}{a+1}] \times [1-E]$	$m''_{0,1} = \frac{\mu_1}{2J_1(\mu_1)} J_0(\mu_1\Phi^{1/2})[1-E]$ $m''_{a,1} = (\frac{2+\frac{1}{2}e^2a^{1/a}}{a+2}) [\frac{J_0(\mu_1\Phi^{1/2})}{a+1} + \frac{a(1-\Phi)}{a+1}] \times [1-E]$	$m''_{0,2} = \frac{\pi^2}{3} \frac{\sin(\pi\Phi^{1/3})}{\pi\Phi^{1/3}}$ $m''_{a,2} = (\frac{2+\frac{1}{2}e^{8/3}a^{1/a}}{a+2}) [\frac{\sin(\pi\Phi^{1/3})}{(a+1)(\pi\Phi^{1/3})} + \frac{a(1-\Phi^{2/3})^{\frac{1}{a+1}}}{a+1}] \times [1-E]$
Transition region with: $m_{a,v} = \frac{(E_R - E)m'_{a,v} + (E - E_T)m''_{a,v}}{E_R - E_T}$ ($E_T \leq E \leq E_R$)		
$E_T = \begin{cases} 1 - \frac{2}{\pi} & (a=0) \\ 1 - (\frac{2+\frac{1}{2}e^2a^{1/a}}{a+2})^{-1/a} & \end{cases}$ $E_R = \frac{1}{a+2}$	$E_T = \begin{cases} 1 - \frac{2J_1(\mu_1)}{\mu_1} & (a=0) \\ 1 - (\frac{2+\frac{1}{2}e^2a^{1/a}}{a+2})^{-1/a} & \end{cases}$ $E_R = \begin{cases} 1 - \frac{J_1(\mu_1)}{\pi\mu_1} & (a=0) \\ 1 - (\frac{2+\frac{1}{2}e^2a^{1/a}}{2+e\cdot a})^{\frac{1}{a+1}} & \end{cases}$	$E_T = \begin{cases} 1 - \frac{3}{\pi^2} & (a=0) \\ 1 - (\frac{2+\frac{1}{2}e^{8/3}a^{1/a}}{a+2})^{-1/a} & \end{cases}$ $E_R = \begin{cases} 1 - \frac{3}{4\pi} & (a=0) \\ 1 - (\frac{2+\frac{1}{2}e^2a^{1/a}}{2+\frac{1}{2}e^{8/3}a})^{\frac{1}{a+1}} & \end{cases}$

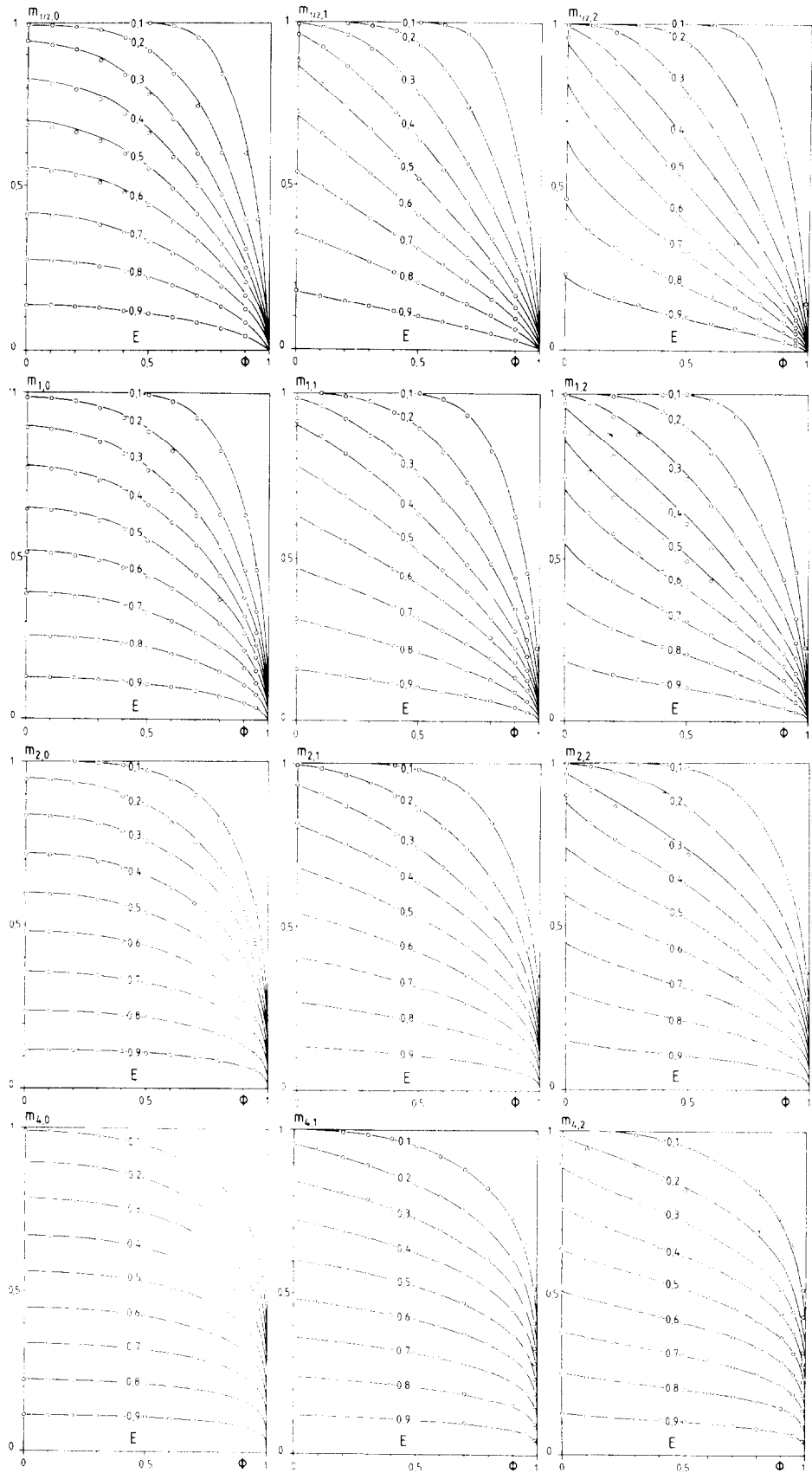


FIG. 4. Concentration profiles $m_{a,v}$ at different values of the efficiency E , for slab ($v = 0$), non-shrinking cylinder ($v = 1$) and non-shrinking sphere ($v = 2$) with $a = \frac{1}{2}, 1, 2, 4$. (—): numerical, (○): approximations according to Table 1.

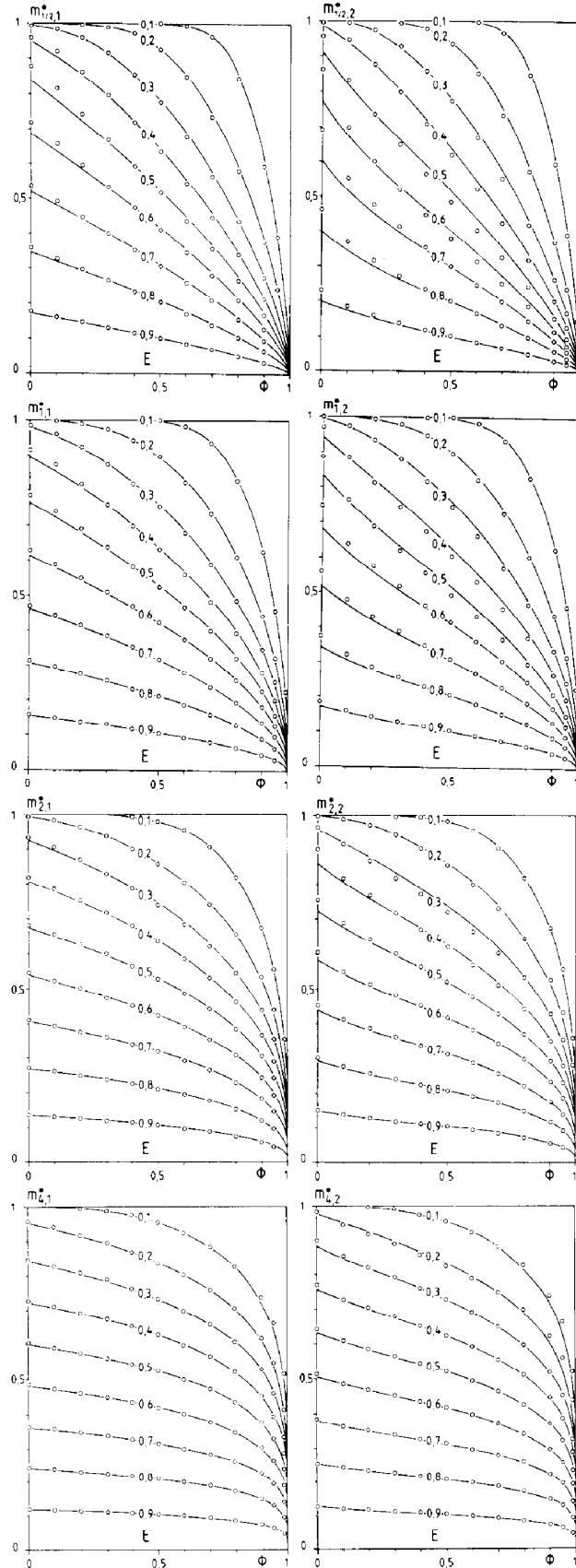


FIG. 5. Concentration profiles $m_{a,v}^*$ at different values of the efficiency E , for a shrinking cylinder ($v = 1$) and sphere ($v = 2$) with $a = \frac{1}{2}, 1, 2, 4$. (—): numerical, (○): approximations according to Table 1.

value of the efficiency in point R is then determined by

$$E_R = 1 - \frac{\bar{g}_{r,a,v}}{\bar{g}_{r,a,0}} \left(\frac{a+1}{a+2} \right). \quad (43)$$

Having established the location of the transition region, we will now turn to the problem of how the transition will take place. We therefore assumed a linear combination between the two limiting approximations, which, anticipating the computational results, appeared to provide an effective transition. The concentration during the transition is then expressed by

$$m_{a,v} = \frac{(E_R - E)m'_{a,v} + (E - E_T)m''_{a,v}}{E_R - E_T} \quad (44)$$

where $m'_{a,v}$ and $m''_{a,v}$ are the short and large time approximations respectively. In Table 1 a summary is presented of the formulas, needed for the computation of concentration profiles in the regions of interest.

3. RESULTS AND DISCUSSION

A numerical solution of equation (1), subject to the boundary conditions as stated in part I, was obtained by a finite difference method, applying the Crank–Nicolson discretization scheme and a variable implicitness factor [2–4]. The approximate concentration profiles were computed according to the relations from Table 1 combined with the procedure for the computation of desorption times as given in part I.

In Fig. 4 the results of both numerical and approximate method are shown for slab, cylinder and sphere at increasing values of a , demonstrating a remarkable agreement. The deviations are mainly located in the transition region, but vanish rapidly as soon as the regular regime and consequently, the large time approximation becomes dominating.

and the diffusion process is virtually proceeding in the regular regime and consequently, the large time approximation becomes dominating.

For shrinking systems, the concentration profiles seem to be only slightly affected by shrinkage, which evidently is inherent in the application of the shrinking coordinate system as defined in part I.

In Fig. 5 we plotted the approximate concentration profiles for shrinking cylinder and sphere together with the profiles obtained numerically. As may be observed, the concentration profiles in case of shrinkage, tend to a slightly more rectangular shape compared to the profiles when no shrinkage is involved. However, as the value of a increases, the occurring differences gradually vanish. From these observations we may conclude that also for shrinking systems the approximate relations from Table 1 can be applied directly for the computation of concentration profiles. Incidentally, it should be pointed out that, although the profiles for shrinking and non-shrinking systems show an apparent similarity for equal values of the efficiency E , the time scale of the diffusion process in both systems is entirely different.

Altogether, the combined methods from parts I and II provide adequate approximations for the solution of the nonlinear diffusion equation, subject to Dirichlet boundary conditions and a power-function variation of the diffusion coefficient with concentration. The approximations cover the three basic geometries: slab, cylinder and sphere and are applicable to systems with or without shrinkage.

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APPENDIX A

THE LARGE TIME SOLUTION FOR A SLAB

For a slab ($v = 0$), equation (4) may be written as

$$\frac{d}{d\phi} \left(g_r^a \frac{dg_r}{d\phi} \right) = -P_{a,0} g_r \quad (A1)$$

subject to the boundary conditions

$$g_r = 1, \quad \frac{dg_r}{d\phi} = 0 \quad \text{at} \quad \phi = 0, \quad (A2)$$

$$g_r = 0 \quad \text{at} \quad \phi = 1. \quad (A3)$$

Multiplying both sides of equation (A1) by $2g_r^a dg_r/d\phi$ and subsequent integration yields

$$g_r^a \frac{dg_r}{d\phi} = \left(\frac{2P_{a,0}}{a+2} \right)^{1/2} (1 - g_r^{a+2})^{1/2}. \quad (A4)$$

Substituting $z = g_r^{a+2}$ in equation (A4) and integrating once more results in

$$[2(a+2)P_{a,0}]^{1/2} (1 - \phi) = \int_0^z z^{-1/(a+2)} (1 - z)^{-1/2} dz. \quad (A5)$$

The RHS of equation (A5) is the integral representation of the incomplete beta function $B_z[(a+1)/(a+2), 1/2]$ [9]. Because at $\phi = 0$, $z = 1$, we obtain from equation (A5)

$$[2(a+2)P_{a,0}]^{1/2} = B\left(\frac{a+1}{a+2}, \frac{1}{2}\right) \quad (A6)$$

where B represents the beta function.
From equation (A6) follows:

$$P_{a,0} = \frac{B^2\left(\frac{a+1}{a+2}, \frac{1}{2}\right)}{2(a+2)} \quad (A7)$$

whereas, equation (A5) turns into

$$B_z\left(\frac{a+1}{a+2}, \frac{1}{2}\right) = B\left(\frac{a+1}{a+2}, \frac{1}{2}\right)(1-\phi) \quad (A8)$$

which, implicitly gives g_r as a function of ϕ .

APPENDIX B

POLYNOMIAL AND RATIONAL APPROXIMATIONS FOR THE FUNCTIONS: $J_0(z)$, $\operatorname{erfc}(z)$ AND $K_{1/4}(z)$ [9]

The Bessel function of order 0: $J_0(z)$ ($-3 \leq z \leq 3$)

$$J_0(z) = 1 - 2.2499997(z/3)^2 + 1.2656208(z/3)^4 - 0.3163866(z/3)^6 + 0.0444479(z/3)^8 - 0.0039444(z/3)^{10} - 0.0002100(z/3)^{12} + |\varepsilon| \quad (B1)$$

with $|\varepsilon| < 5 \times 10^{-8}$.

The complementary error function: $\operatorname{erfc}(z)$

$$\operatorname{erfc}(z) = (0.254829592x - 0.284496736x^2 + 1.421413741x^3 - 1.453152027x^4 + 1.061405429x^5)e^{-z^2} + |\varepsilon| \quad (B2)$$

with

$$x = 1/(1 + 0.3275911z) \quad \text{and} \quad |\varepsilon| \leq 1.5 \times 10^{-7}.$$

The modified Bessel function of order $\frac{1}{4}$: $K_{1/4}(z)$: Approximation for large values of z

$$K_{1/4}(z) = (\pi/2z)^{1/2} e^{-z} \left[1 - \frac{0.75}{8z} + \frac{(0.75)(8.75)}{2(8z)^2} - \frac{(0.75)(8.75)(24.75)}{6(8z)^3} \right] \quad (B3)$$

UNE METHODE APPROCHEE DE RESOLUTION DU PROBLEME DE DIFFUSION NON LINEAIRE AVEC UNE LOI PUISSANCE ENTRE LE COEFFICIENT DE DIFFUSION ET LA CONCENTRATION—II. CALCUL DES PROFILS DE CONCENTRATION

Résumé—La méthode approchée développée dans la partie I [1] est étendue avec des relations approchées pour le calcul des profils de concentration dans un mécanisme de désorption non linéaire avec des conditions aux limites de Dirichlet et une variation en loi puissance du coefficient de diffusion en fonction de la concentration. Les relations sont applicables aux systèmes rétractables ou non à géométrie plane, cylindrique ou sphérique.

EINE NÄHERUNGSMETHODE ZUR LÖSUNG DES NICHTLINEAREN DIFFUSIONSPROBLEMS MIT EINER POTENZBEZIEHUNG ZWISCHEN DIFFUSIONSKOEFFIZIENT UND KONZENTRATION—II. BERECHNUNG VON KONZENTRATIONSPROFILIEN

Zusammenfassung—Die in Teil I [1] entwickelte Näherungsmethode wird erweitert durch Näherungsbeziehungen für die Berechnung von Konzentrationsprofilen für einen nichtlinearen Desorptionsprozeß mit Dirichlet-Randbedingungen und einer Veränderung des Diffusionskoeffizienten mit der Konzentration nach einer Potenzfunktion. Die Beziehungen sind anwendbar auf nicht-schrumpfende oder schrumpfende Systeme mit Platten-, Zylinder- bzw. Kugengeometrie.

ПРИБЛИЖЕННЫЙ МЕТОД РЕШЕНИЯ ЗАДАЧА НЕЛИНЕЙНОЙ ДИФФУЗИИ ПРИ СТЕПЕННОЙ ЗАВИСИМОСТИ КОЭФФИЦИЕНТА ДИФФУЗИИ ОТ КОНЦЕНТРАЦИИ. II. РАСЧЕТ ПРОФИЛЕЙ КОНЦЕНТРАЦИИ

Аннотация — Проводится некоторая модификация предложенного в работе [I] приближенного метода, который затем используется для расчета профилей концентрации нелинейного процесса десорбции при граничных условиях Дирихле и степенной зависимости коэффициента диффузии от концентрации. Метод может применяться для расчета систем с усадкой или без в случае следующих геометрий: пластина, цилиндр, шар.