Exact analytical solution of a nonlinear reaction–diffusion model in porous catalysts

Eugen Magyari *

Institut für Hochbautechnik, ETH Zürich, Wolfgang-Pauli-Str. 1, CH-8093 Zürich, Switzerland

ARTICLE INFO

ABSTRACT

In two papers published recently in Chemical Engineering Journal, [Y.P. Sun, S.B. Liu, S. Keith, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by decomposition method, Chem. Eng. J. 102 (2004) 1–10; S. Abbasbandy, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by means of the homotopy analysis method, Chem. Eng. J. 136 (2008) 144–150], a nonlinear model of diffusion and reaction in porous catalysts has been investigated by approximate analytical methods (the Adomian decomposition method, [Y.P. Sun, S.B. Liu, S. Keith, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by decomposition method, Chem. Eng. J. 102 (2004) 1–10] and the homotopy analysis method, [S. Abbasbandy, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by means of the homotopy analysis method, Chem. Eng. J. 136 (2008) 144–150], respectively). The present paper shows, however, that the model is exactly solvable in terms of Gauss' hypergeometric function. The exact solution is illustrated by specific examples. Several new physical features are reported and discussed in detail.

© 2008 Elsevier B.V. All rights reserved.

1. Introduction and problem formulation

The aim of the present paper is to give the exact analytical solutions of a nonlinear diffusion-reaction model investigated in the recent literature extensively by different approximation methods [1,2].

The model considered by Sun et al. [1] and Abbasbandy [2] describes the *steady* diffusion-reaction regime in a porous slab with plane boundaries at $X = 0$ and $X = L$, respectively. The concentration distribution of the reactant, $C = C(X)$ satisfies the differential equation

$$D_e \frac{d^2 C}{dX^2} - r(C) = 0 \tag{1}$$

where the reaction rate per unit volume r is a power law function of the concentration,

$$r = kC^n \tag{2}$$

The admitted range of the reaction order is $n \geq -1$. The boundary at $X = 0$ is impermeable (vanishing mass flux) and that at $X = L$ is held

at a constant concentration C_S,

$$D_e \left. \frac{dC}{dX} \right|_{X=0} = 0, \quad C|_{X=L} = C_S \tag{3}$$

In terms of the dimensionless variables

$$x = \frac{X}{L}, \quad c(x) = \frac{C(X)}{C_S} \tag{4}$$

the boundary value problems (1)–(3) is specified by equations

$$\frac{d^2 c}{dx^2} - \phi^2 c^n = 0 \tag{5}$$

$$\left. \frac{dc}{dx} \right|_{x=0} = 0, \quad c|_{x=1} = 1 \tag{6}$$

where $\phi = (kL^2 C_S^{n-1}/D_e)^{1/2}$ denotes the Thiele modulus.

Approximate series solutions of the one-dimensional nonlinear boundary value problem (5), (6) have been given recently for different values of the parameters n and ϕ with the aid of Adomian's decomposition method and the homotopy analysis method by Sun et al. [1] and by Abbasbandy [2], respectively. The present paper gives the exact analytical solutions in terms of Gauss' hypergeometric function. For a comprehensive review of more general reaction diffusion problems in porous catalysis, see e.g. Ref. [3].

* Tel.: +41 61 731 38 46.
  E-mail addresses: magyari@hbt.arch.ethz.ch, magyari@bluewin.ch.

Nomenclature

c	dimensionless concentration
C	concentration
C_S	prescribed concentration at $X = L$
D_e	effective diffusion coefficient
F	Gauss' hypergeometric function
k	reaction rate constant
K	integration constant
L	thickness of porous slab
m	$n + 1$
n	reaction order
q_M	mass flux at $X = L$
r	reaction rate per unit volume
u	variable of integration
x	dimensionless transversal coordinate
X	transversal coordinate

Greek symbols

Γ	Euler's Gamma function
ϕ	$= (kL^2 C_S^{n-1}/D_e)^{1/2}$, Thiele modulus

Subscript/superscript

Prime	differentiation with respect to x
0	at the boundary $x = 0$

2. The exact solution for $n > -1$

One easily sees that Eq. (5) admits the first integral

$$\frac{1}{2}\left(\frac{dc}{dx}\right)^2 - \frac{\phi^2}{m}c^m = K \tag{7}$$

where K is a constant of integration and $m = n + 1$. Eq. (7) holds for all $n \neq -1$. The case $n = -1$ will be discussed in Section 3.2.

The first boundary condition (6) and Eq. (7) give for the integration constant K the value

$$K = -\frac{\phi^2}{m}c_0^m \tag{8}$$

where $c_0 = c(0)$ denotes the (yet unknown) concentration of the reactant at the impermeable boundary of the porous slab, and represents one of the quantities of main engineering interest of the problem. Thus, Eq. (7) becomes

$$\left(\frac{dc}{dx}\right)^2 = \frac{2\phi^2}{m}(c^m - c_0^m) \tag{9}$$

and yields

$$x = \frac{1}{\phi}\left(\frac{m}{2c_0^{m-2}}\right)^{1/2}\int_1^{c/c_0}\frac{du}{\sqrt{u^m-1}} \quad (m \neq 0) \tag{10}$$

Using the software package of *Mathematica®*, the integral in Eq. (10) can be expressed in terms of Gauss' hypergeometric function $F \equiv {}_2F_1(a,b; c; z)$ as follows:

$$\int_1^u \frac{du}{\sqrt{u^m-1}} = \frac{2}{2-m}\left[u^{1-m/2}F\left(\frac{1}{2}-\frac{1}{m},\frac{1}{2};\ \frac{3}{2}-\frac{1}{m};\ u^{-m}\right)\right.$$
$$\left. - F\left(\frac{1}{2}-\frac{1}{m},\frac{1}{2};\ \frac{3}{2}-\frac{1}{m};\ 1\right)\right] \tag{11}$$

For a comprehensive description of the hypergeometric function F, see e.g. [4], Chap. 15. With the aid of Eqs. (15.3.6) and (15.1.8) of
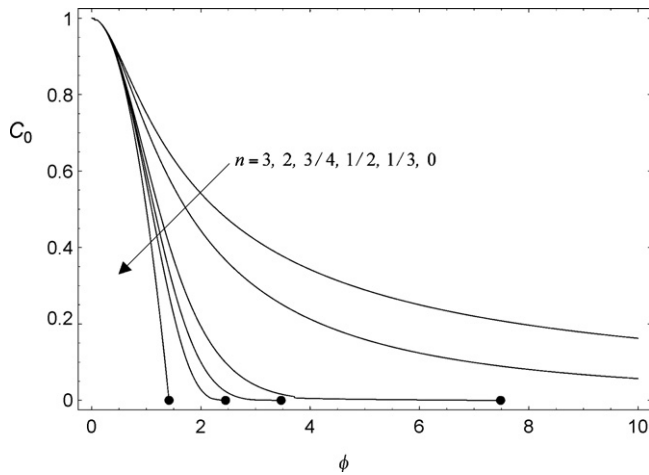
Ref. [4], Eq. (11) can be transcribed into form

$$\int_1^u \frac{du}{\sqrt{u^m-1}} = \frac{2}{m}u^{1-m}(u^m-1)^{1/2}F\left(1,1-\frac{1}{m};\ \frac{3}{2};\ 1-u^{-m}\right) \tag{12}$$

and thus, the exact solution of the problem is obtained in the implicit form

$$x = \frac{1}{\phi}\left(\frac{2}{mc_0^{m-2}}\right)^{1/2}\left(\frac{c}{c_0}\right)^{1-m}\left[\left(\frac{c}{c_0}\right)^m - 1\right]^{1/2}$$
$$\times F\left(1, 1-\frac{1}{m};\ \frac{3}{2};\ 1-\left(\frac{c}{c_0}\right)^{-m}\right) \tag{13}$$

Now, the concentration c_0 at the impermeable boundary of the porous slab can be determined from the exact solution (13) and the second boundary condition (6) as solution of the transcendental equation

$$\frac{1}{\phi}\left[\frac{2}{m}(1-c_0^m)\right]^{1/2}F\left(1, 1-\frac{1}{m};\ \frac{3}{2};\ 1-c_0^m\right) = 1 \tag{14}$$

In addition to c_0, a further quantity of engineering interest of the present problem is the mass flux

$$q_M = -D_e\left.\frac{dC}{dX}\right|_{X=L} = -\frac{D_e C_S}{L}\left.\frac{dc}{dx}\right|_{x=1} \tag{15}$$

through the boundary $X = L$ where the constant concentration C_S was prescribed. This *ingoing* mass flux is necessary in order to maintain the *steady* reaction regime during the consumption of the reactant in the chemical reaction. The dimensionless concentration gradient $dc/dx|_{x=1} \equiv c'(1)$ occurring in Eq. (15) is obtained by differentiation of Eq. (13) in the form

$$c'(1) = \frac{(m/2)^{1/2}\phi}{\begin{array}{c}\left(m+2(1-m)(1-c_0^m)/2(1-c_0^m)^{1/2}F\right)(1, 1-1/m;\ 3/2;\ 1-c_0^m)\\+(2(1-m)/3)c_0^m(1-c_0^m)^{1/2}F(2, 2-1/m;\ 5/2;\ 1-c_0^m)\end{array}} \tag{16}$$

The equivalent expression of $c'(1)$,

$$c'(1) = \left[1-m+\frac{m}{2(1-c_0^m)}+\frac{2(1-m)}{3\phi}c_0^m\left[\frac{2}{m}(1-c_0^m)\right]^{1/2}\right.$$
$$\left. \times F\left(2, 2-\frac{1}{m};\ \frac{5}{2};\ 1-c_0^m\right)\right]^{-1} \tag{17}$$

results from Eqs. (14) and (16) easily. From geometrical point of view, the value of $c'(1)$ represents the slope of the dimensionless concentration profile $c = c(x)$ at the boundary $x = 1$.

3. Discussion

The main advantage of the exact analytical solution (13) consists of the facts that (i) the mathematical properties of the hypergeometric function F are well established (see e.g. Ref. [4]) and (ii) today, well-performing commercial computer software is available both for symbolical and numerical calculations involving the function F (in the present paper throughout Wolfram's *Mathematica®* has been used). This circumstance facilitates both the analytical and numerical investigation of the concentration distribution $c = c(x)$ substantially (without to be confronted with the convergence problems arising in approximation methods). In the following, the features of the solution $c = c(x)$ will be examined for positive and negative values of the reaction order in the range $n \geq -1$.

Fig. 1. Plot of the concentration c_0 at the impermeable wall as function of the Thiele modulus ϕ for six nonnegative values of the reaction order n. The dots mark the maximum values $\phi^*(n)$ of ϕ where $c_0 = 0$ when $0 \leq n < 1$. These values are: $\phi^*(0) = \sqrt{2} = 1.41$, $\phi^*(1/3) = \sqrt{6} = 2.45$, $\phi^*(1/2) = 2\sqrt{3} = 3.46$ and $\phi^*(3/4) = 7\sqrt{14} = 7.48$, respectively.

3.1. Positive and vanishing reaction orders, $n \geq 0$

To get a first insight into the domain of existence of solutions, in Fig. 1 the dependence of the surface concentration $c_0 = c(0)$ on the Thiele modulus ϕ has been plotted for six different values of the reaction order n according to Eq. (14).

An inspection of Fig. 1 emphasizes three remarkable features, namely:

(i) The surface concentration c_0 decreases monotonously with increasing values of the Thiele modulus for all $n \geq 0$.
(ii) The function $c_0 = c_0(\phi; n)$ approaches unity for all $n \geq 0$ as $\phi \to 0$.
(iii) In the range $0 \leq n < 1$, the curves $c_0 = c_0(\phi; n)$ terminate at some finite values $\phi^*(n)$ of ϕ, where the concentration c_0 goes to zero (while for $n > 1$, $c_0 = c_0(\phi; n)$ approaches zero only as $\phi \to \infty$). In other words, the domain of existence of solutions in the range $0 \leq n < 1$ is $0 \leq \phi \leq \phi^*(n)$.

The property (ii) is a direct consequence of the fact that the boundary value problem (5) and (6) admits for $\phi = 0$ the constant solution

$$c(x) = 1 \qquad (\phi = 0) \tag{18}$$

for all n. The existence of the maximum value $\phi^*(n)$ of ϕ where $c_0 = 0$, as mentioned under point (iii), can rigorously be proven by taking the limit $c_0 \to 0$ of the exact analytical results (13) and (14). In this way, bearing in mind Eq. (15.1.20) of [4], one obtains that

$$c(x) = x^{2/1-n} \tag{19}$$

is an exact solution of the boundary value problem (5) and (6) when

$$\phi = \frac{\sqrt{2(1+n)}}{1-n} \equiv \phi^*(n) \quad \text{and} \quad -1 < n < 1 \tag{20}$$

The latter condition (20) ensures that in this case $c_0 = c(0) = 0$. The results (19) and (20) can also be proven easily by a direct substitution in Eqs. (5) and (6).

For the dimensionless concentration gradient at the boundary $x = 1$ one obtains in this case from Eq. (17)

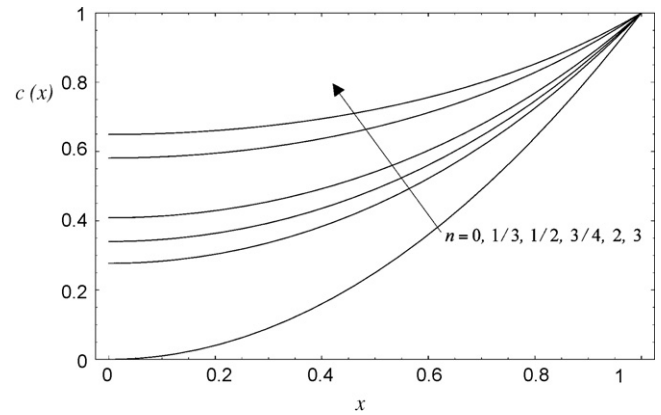$$c'(1) = \frac{2}{1-n} \quad (-1 < n < 1) \tag{21}$$

Fig. 2. Concentration profiles plotted as functions of the coordinate x, for $\phi = \sqrt{2}$ and six different values of the reaction order n. The corresponding concentrations at the impermeable wall are $c_0 = 0, 0.277164, 0.340257, 0.408617, 0.581345$ and 0.649268, respectively.

As an illustration, in Fig. 2 the concentration profiles $c = c(x)$ given by the exact solution (13) have been plotted for the reaction orders $n = 0$, 1/3, 1/2, 3/4, 2 and 3 and the same value $\phi = \sqrt{2}$ of the Thiele modulus. The value $\phi = \sqrt{2}$ coincides according to Eq. (20) with the maximum value $\phi^*(n)$ for $n = 0$. Accordingly, in this case one has $c(x) = x^2$ and $c_0 = 0$. For the other reaction orders, $n = 1/3$, 1/2, 3/4, 2 and 3, the concentrations at the impermeable wall are $c_0 = 0.277164, 0.340257, 0.408617, 0.581345$ and 0.649268, respectively. For the slopes of the concentration profiles shown in Fig. 2, Eqs. (19) and (17) yield the values $c'(1) = 2$ for $n = 0$ and $c'(1) = 1.56776, 1.46198, 1.34476, 1.03507$ and 0.906805 for $n = 1/3$, 1/2, 3/4, 2 and 3, respectively. One sees that, the smaller the reaction order n, the steeper the concentration profile in the neighborhood of the boundary $x = 1$.

Taking into account that

$$F(a, 0; \ c; \ z) = 1, \tag{22}$$

Eq. (13) gives for $n = 0$ (i.e. $m = 1$) the explicit solution

$$c(x) = c_0 + \frac{\phi^2}{2}x^2 \qquad (n = 0) \tag{23}$$

Eq. (14) yields for c_0 the value

$$c_0 = 1 - \frac{\phi^2}{2} \qquad (n = 0) \tag{24}$$

Therefore, the domain of existence of the solution (23) is $0 \leq \phi \leq \phi^*(0) = \sqrt{2}$, in agreement with Eq. (20) and Fig. 1.

A further case in which the general exact solution (13) reduces to an elementary form is the case of first order reactions, $n = 1$, where the boundary value problem (5) and (6) becomes linear. Bearing in mind that for $n = 1$ (i.e. $m = 2$) one has [4]

$$F\left(1, 1 - \frac{1}{m}; \ \frac{3}{2}; \ 1 - \left(\frac{c}{c_0}\right)^{-m}\right) = F\left(1, \frac{1}{2}; \ \frac{3}{2}; \ 1 - \left(\frac{c_0}{c}\right)^2\right)$$

$$= \frac{\operatorname{arctanh}\sqrt{1 - (c_0/c)^2}}{\sqrt{1 - (c_0/c)^2}}, \tag{25}$$

Eq. (13) reduces to $\phi x = \operatorname{arctanh}\sqrt{1 - (c_0/c)^2}$. In this way, we recover the well-known elementary solution

$$c(x) = c_0 \cosh(\phi x) \tag{26}$$

The second boundary condition (6) yields for c_0 the value

$$c_0 = \frac{1}{\cosh \phi} \tag{27}$$

Table 1
Special cases of the exact solution for four negative values of the apparent reaction order in the range $-1 < n < 0$

n	$m = n + 1$	Eq. (13)
$-\frac{1}{3}$	$\frac{2}{3}$	$x = \frac{\sqrt{3}c_0^{2/3}}{2\phi}\left[\left(\frac{c}{c_0}\right)^{1/3}\sqrt{\left(\frac{c}{c_0}\right)^{2/3}-1} - \text{arccosh}\left(\frac{c}{c_0}\right)^{1/3}\right]$
$-\frac{1}{2}$	$\frac{1}{2}$	$x = \frac{2c_0^{3/4}}{3\phi}\left(\sqrt{\frac{c}{c_0}}-1\right)^{1/2}\left(\sqrt{\frac{c}{c_0}}+2\right)$
$-\frac{2}{3}$	$\frac{1}{3}$	$x = \frac{c_0^{5/6}}{5\phi}\sqrt{\frac{2}{3}}\sqrt{\left(\frac{c}{c_0}\right)^{1/3}-1}\left[8+4\left(\frac{c}{c_0}\right)^{1/3}+3\left(\frac{c}{c_0}\right)^{2/3}\right]$
$-\frac{3}{4}$	$\frac{1}{4}$	$x = \frac{2\sqrt{2}c_0^{7/8}}{35\phi}\sqrt{\left(\frac{c}{c_0}\right)^{1/4}-1}\left[16+8\left(\frac{c}{c_0}\right)^{1/4}+6\left(\frac{c}{c_0}\right)^{1/2}+5\left(\frac{c}{c_0}\right)^{3/4}\right]$

while the dimensionless mass flux $c'(1) = dc/dx|_{x=1}$ through the boundary at $x = 1$ is obtained from Eq. (16) and (27) as

$$c'(1) = \phi \tanh \phi \tag{28}$$

We mention that, in addition to the elementary solutions (19) and (26) associated with nonnegative values of n, in the range $-1 \leq n < 0$ from the exact solution (13) further elementary solutions can be obtained (see Section 3.2).

In order to compare the exact solutions (13) to the approximate series solutions of Refs. [1] and [2], one has first to expand the right hand side of Eq. (13) in a Taylor series to $(c-c_0)$ and then, to invert this power series to the explicit form $c = c(x)$. Using a the algebra software of *Mathematica®*, this procedure led us to the result

$$c(x) = c_0 + c_0^n\frac{(\phi x)^2}{2!} + nc_0^{2n-1}\frac{(\phi x)^4}{4!} + n(4n-3)c_0^{3n-2}\frac{(\phi x)^6}{6!}$$
$$+ n(34n^2 - 63n + 30)c_0^{4n-3}\frac{(\phi x)^8}{8!} + n(496n^3 - 1554n^2$$
$$+ 1689n - 630)c_0^{6n-5}\frac{(\phi x)^{10}}{10!} + \cdots \tag{29}$$

As expected, for $n = 0$ one recovers in Eq. (29) the exact solution (23) and for $n = 1$ the series expansion of the elementary solution (26),

$$c(x) = c_0\left(1 + \frac{(\phi x)^2}{2!} + \frac{(\phi x)^4}{4!} + \frac{(\phi x)^6}{6!} + \frac{(\phi x)^8}{8!} + \frac{(\phi x)^{10}}{10!} + \cdots\right) \tag{30}$$

The expansion (29) coincides with the result of Abbasbandy, [2], exactly. It also coincides with Eq. (26) of [1], except for the coefficients of $(\phi x)^6$ and $(\phi x)^8$ which have been affected in [1] by typos.

3.2. Negative reaction orders n

Eq. (12), and consequently the exact solution (13) apply for all $m = n + 1 > 0$, i.e. for all $n > -1$. However, for $m = 0$ (i.e. $n = -1$), Eq. (13) as well as the first integral (7) become infinite, as already mentioned in Section 2. This case requires a special approach and will be considered separately at the end of the present section, after the subsequent discussion of the apparent reaction order range $-1 < n < 0$.

The range $-1 < n < 0$ (i.e. $0 < m < 1$)

In the range of apparent reaction order $-1 < n < 0$ the exact solution (13) reduces in several special cases to elementary transcendental functions. Four of such cases (calculated with the aid of *Mathematica®*) are collected in Table 1. The concentrations c_0 at the impermeable wall as functions of the Thiele modulus ϕ are plotted for the cases included in Table 1 in Fig. 3.
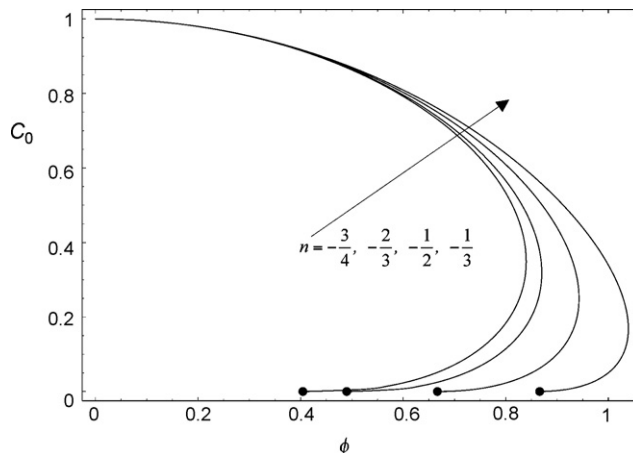

Fig. 3. Plot of the concentration c_0 at the impermeable wall as function of the Thiele modulus ϕ for four negative values of the reaction order in the range $-1 < n < 0$.

A comparison of Fig. 3 (where $-1 < n < 0$) to Fig. 1 (where $n > 0$) indicates dramatic differences which can be described as follows:

(i) In the range $-1 < n < 0$ the surface concentration c_0 is no longer a monotonous function of the Thiele modulus ϕ.
(ii) For every reaction order in the range $-1 < n < 0$, there exists a maximum value $\phi_{\max}(n)$ so that the boundary value problem (5), (6) does not admit solutions for $\phi > \phi_{\max}(n)$.
(iii) The surface concentration c_0 reaches at $\phi > \phi_{\max}(n)$ a critical value $c_{0,\text{crit}}(n)$ which represents a turning point of the function $c_0 = c_0(\phi; n)$.
(iv) The curves $c_0 = c_0(\phi; n)$ terminate at some finite values $\phi^*(n)$ of ϕ. The values of $\phi^*(n)$ are given by Eq. (20).
(v) While in the ranges $0 \leq \phi < \phi^*(n)$ the solutions of the boundary value problem (5) and (6) are unique, in the ranges $\phi^*(n) \leq \phi \leq \phi_{\max}(n)$ two solution branches (*dual solutions*) occur.
(vi) At $\phi = \phi^*(n)$, one of the dual solutions corresponds to the surface concentration $c_0 = 0$ (lower branch) and the another to $c_0 = c^*(n)$ (upper branch), respectively. In the former case the concentration distribution is given by Eq. (19).
(vii) At the turning point $(\phi, c_0) = (\phi_{\max}, c_{0,\text{crit}})$, the dual solutions become coincident.

For the reaction orders selected in Table 1 and Fig. 3, the above characteristic quantities are given in Table 2.

The case $n = -1$ (i.e. $m = 0$)

Eq. (5) admits also for $n = -1$ a first integral which has now the form

$$\frac{1}{2}\left(\frac{dc}{dx}\right)^2 - \phi^2 \ln c = K \tag{31}$$

Table 2
Characteristics of the exact solutions for the cases selected in Table 1 and plotted in Fig. 3

n	$\phi^*(n)$	$c^*(n)$	$\phi_{\max}(n)$	$c_{0,\text{crit}}(n)$	$c(x)$, Eq. (19)
$-1/3$	$\sqrt{3}/2 = 0.87$	0.562573	1.03895	0.168594	$x^{3/2}$
$-1/2$	$2/3 = 0.67$	$3/4 = 0.75$	0.942809	$1/4 = 0.25$	$x^{4/3}$
$-2/3$	$\sqrt{5}/6 = 0.49$	0.870468	0.870131	0.318629	$x^{6/5}$
$-3/4$	$2\sqrt{2}/7 = 0.40$	0.913653	0.839768	0.348775	$x^{8/7}$

The concentration distributions $c(x)$ of the last column correspond to $c_0 = 0$ and $\phi = \phi^*(n)$.
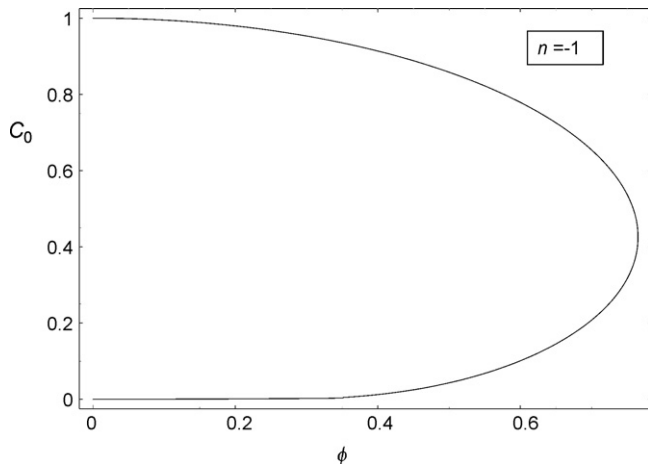
Fig. 4. Plot of the concentration c_0 as function of ϕ for $n = -1$. There exist dual solutions only. Their domain of existence is $0 \leq \phi \leq \phi_{\max}(-1) = 0.765152$. The critical value of c_0, where the lower and upper branch solutions become coincident is $c_{0,\max} = 0.425695$.

The first boundary condition (6) and Eq. (31) give for the integration constant K the value $K = -\phi^2 \ln c_0$. Thus, Eq. (31) becomes

$$\left(\frac{dc}{dx}\right)^2 = 2\phi^2 \ln\left[\frac{c(x)}{c_0}\right] \tag{32}$$

and yields the exact solution of the problem in the implicit analytical form

$$x = \frac{c_0}{\phi\sqrt{2}} \int_1^{c/c_0} \frac{du}{\sqrt{\ln u}} = \frac{c_0}{i\phi}\sqrt{\frac{\pi}{2}}\,\mathrm{erf}\left[i\sqrt{\ln\left(\frac{c}{c_0}\right)}\right] \tag{33}$$

In Eq. (33), $\mathrm{erf}(z)$ denotes the error function [4].

The concentration c_0 at the impermeable boundary can be determined from the exact solution (33) and the second boundary condition (6) as solution of the transcendental equation

$$\frac{c_0}{i\phi}\sqrt{\frac{\pi}{2}}\,\mathrm{erf}\left[i\sqrt{\ln\left(\frac{1}{c_0}\right)}\right] = 1 \tag{34}$$

The dimensionless concentration gradient $dc/dx|_{x=1} \equiv c'(1)$ at the boundary with prescribed concentration is obtained by differentiation of Eq. (33) in the form

$$c'(1) = \phi\sqrt{-2\ln c_0} \tag{35}$$

The concentration c_0 at the impermeable wall as function of the Thiele modulus ϕ is plotted according to Eq. (34) in Fig. 4.

The curve $c_0 = c_0(\phi; -1)$ of Fig. 4 bears a close resemblance to the curves of Fig. 3 corresponding to reaction orders in the range $-1 < n < 0$. An essential difference, however, is that its lower branch does not terminate at a finite value ϕ^* of the Thiele modulus, but $\phi^*(-1) \to 0$ as $c_0 \to 0$. Accordingly, for $n = -1$ no unique solutions exist al all, except at the critical value $c_{0,\max} = 0.425695$ of c_0, where the lower and upper branch solutions become coincident. The domain of existence of the dual solution in this case is $0 \leq \phi \leq \phi_{\max}(-1) = 0.765152$. The shape of concentration profiles $c = c(x; \phi; n)$ is qualitatively similar in the whole range $-1 \leq n < 0$ to those corresponding to $n \geq 0$, namely, for any specified value of ϕ in the domain of existence, the local concentration increases from c_0 to the value 1 monotonously as x increases from 0 to 1 (see Fig. 2).

4. Summary and conclusions

A one-dimensional nonlinear model of reaction and diffusion in porous catalysts has been revisited in this paper. One of the boundaries of the porous slab is impermeable and the other one is held at constant concentration. The exact analytical solution for the steady concentration field has been given in terms of Gauss' hypergeometric function. Two quantities of engineering interest, namely the (dimensionless) concentration c_0 at the impermeable boundary $x = 0$, and the concentration gradient $c'(1)$ at boundary $x = 1$ with prescribed concentration, have been calculated and discussed as functions of the reaction order $n \geq -1$ and the Thiele modulus $\phi \geq 0$ in detail. The former quantity provides information about the tightness performance of the respective boundary in satisfying the impermeability requirement. The concentration gradient $c'(1)$ on the other hand, specifies the mass flux of the reactant supply, required to maintain the steady reaction–diffusion regime during the (reactant consuming) chemical reaction. The main results of the paper can be summarized as follows:

(1) The steady concentration $c = c(x)$ increases monotonously from c_0 to 1 for all $n \geq -1$ and $\phi \geq 0$ as the transversal coordinate x increases from 0 to 1. However, the domain of existence of these solutions in the parameter plane (c_0, ϕ), as well as their uniqueness, depend essentially on whether the reaction order is negative, $-1 \leq n < 0$ or nonnegative, $n \geq 0$.
(2) In the range $n \geq 0$, the solutions $c = c(x)$ are unique. When $n \geq 1$, one has $c_0 \neq 0$ and the unique solution exists for all $0 \leq \phi < \infty$. However, in the range $0 \leq n < 1$ of the reaction order, the solution $c = c(x)$ does exist only in a finite interval of values $0 \leq \phi \leq \phi^*(n)$ of the Thiele modulus. Within this interval $c_0 \neq 0$, but at its upper bound $\phi = \phi^*(n)$, one has $c_0 = 0$ (see Fig. 1).
(3) In the range $-1 < n < 0$ of the reaction order, the solutions $c = c(x)$ are unique only for the values of the Thiele modulus in the interval $0 \leq \phi < \phi^*(n)$. In the finite range $\phi^*(n) \leq \phi \leq \phi_{\max}(n)$ above of $\phi^*(n)$, two solution branches (*dual solutions*) occur, and for $\phi > \phi_{\max}(n)$ no solutions exist at all. The surface concentration c_0 reaches at $\phi = \phi_{\max}(n)$ a critical value $c_{0,\mathrm{crit}}(n)$ which represents a turning point of the function $c_0 = c_0(\phi; n)$, where the dual solutions become coincident (see Fig. 3).
(4) For $n = -1$ no unique solutions exist al all, except at the critical value $c_{0,\max} = 0.425695$ of c_0, where the lower and upper branch solutions become coincident. The domain of existence of the dual solution in this case is $0 \leq \phi \leq \phi_{\max}(-1) = 0.765152$ and $\phi^*(-1) \to 0$ as $c_0 \to 0$ (see Fig. 4).

We may conclude that the exact analytical solution reported in the present paper allows for a comprehensive description of the basic physical features of the model considered.

References

[1] Y.P. Sun, S.B. Liu, S. Keith, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by decomposition method, Chem. Eng. J. 102 (2004) 1–10.
[2] S. Abbasbandy, Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by means of the homotopy analysis method, Chem. Eng. J. 136 (2008) 144–150.
[3] R. Aris, The mathematical Theory of Diffusion and Reaction in Permeable Catalysts, vol. 1. The Theory of Steady State, Clerendon, Oxford, 1975.
[4] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions, Dover, New York, 1970.