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Research Note on Power-Series Expression of Mass Concentration Profile in Nonlinear Diffusion-Reaction Processes

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Abstract – *In this paper, a steady state one-dimensional diffusion-reaction process is considered. As a descriptive mathematical model for such processes, a high nonlinear boundary value problem (BVP) for a second order ordinary differential equation is associated. By using an opportune integral representation for the solution of such BVP, fundamentals aspects are provided in order to support the existence and uniqueness of a power series expression as solution of the BVP. So that, a contribution has been reached, leading to provide information of practical significance regarding to the mass concentration profile of the key reactant component in the process.* **Copyright © 2011 Praise Worthy Prize S.r.l. - All rights reserved.**

Keywords*: Concentration Profile, Diffusion-Reaction*

I. Introduction

Let us consider the following one dimensional nonlinear boundary value problem:

$$\frac{d^2u}{dx^2} = -\phi^2 F(u),\ \forall x \in [0,1] \tag{1}$$

$$u = 0 \ \ at \ \ x = 0 \tag{2}$$

$$\frac{du}{dx} = 0 \ \ at \ \ x = 1 \tag{3}$$

The BVP (1) – (3) can be considered as a descriptive non-dimensional mathematical model for a steady-state one-dimensional diffusion-reaction phenomena occurring inside of a catalytic porous slab particle supported on the bed of an heterogeneous chemical reactor.

The unknown is the real function $u = u(x)$ of the real spatial variable *x* (*x* = 0 in surface and *x* = 1 in center of the particle). *u*(*x*) denotes $1-U$, beeing *U* the non-dimensional mass concentration profile of the key component in the process, that is, $U = \frac{C}{C_S}$, where C_S is the corresponding surfacial concentration.

The equation (1) comes from the corresponding mass balance in steady state for the key component, which is consumed in the chemical reaction.

$F(u)$ is the kinetic law of the irreversible chemical reaction involved in the process, a nonlinear regular real function. ϕ denotes the classical Thiele Modulus parameter.

The equation (2) means $C = C_S$ on surface, while (3) comes from symmetry considerations.

For thermodinamical and physicochemical aspects, as well as the corresponding model formulation, see [1] and [2].

In general, it is well known that the analytical solution of the BVP (1) - (3) is quite difficult to be obtained. Most of the available results deals with numerical treatment or with applications of some mathematical methods which leads to obtain successive approximations to the respective solution. For an overview we refer to [3], [4], [5], [6] and [7]. In particular, updates of pertinent literature can be seen in [3].

In [8], a power series expression was calculated as theoretical solution of the BVP (1) - (3). Its numerical results were compared with values of available literature, obtaining a very good agreement.

In the present article, fundamentals are presented to support the existence and uniqueness of analytical formulae (given by the power serie expression reported in [8]), as solution of the mentioned BVP. Hence, this work esentially provides theoretical fundaments to the solution already reported there.

II. Equivalent Integral Representation to BVP (1)-(3)

Notice that on the solution $u = u(x)$ to the BVP (1)-(3) it is required that:

$$u \in C^2[0,1],\ 0 \le u(x) \le 1 \quad \forall x \in [0,1] \tag{4}$$

Then, the following integral representation for the solution $u = u(x)$ to such BVP is obtained:

$$u(x) = \phi^2 \int_0^x \left[\int_t^1 F[u(z)]\,dz \right] dt \tag{5}$$

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In addition to the basic requirements consigned by (4), the following condition on the function $F(u)$ in (1) is assumed:

F is a continuously derivative function $\forall u \in [0,1]$ **(H_0)**

So, for all functions $u, v \in V$, with V the normed vectorial space given as:

$$V \equiv \left\{ w \,/\, w \in C^2[0,1], \|w\| = \underset{x\in[0,1]}{Max} |w(x)| \right\} \quad (6)$$

the following inequality holds:

$$\|W(u) - W(v)\| \le L \frac{\phi^2}{2} \|u - v\|, \forall u, v \in V \quad (7)$$

where W denote an integral operator defined as:

$$W(u) = \phi^2 \int_0^x \left[\int_t^1 F[u(z)] dz \right] dt \quad (8)$$

and L is a positive constant which represent the Lipschitz constant of the function F. In view of assumption (**H_0**), L can be taken as given by:

$$L = \underset{u\in[0,1]}{Max} \left| \frac{dF}{du} \right| \quad (9)$$

It can be seen that whenever the following restriction holds:

$$L < \frac{2}{\phi^2} \quad (10)$$

W result to be a contractive operator. Consequently, the existence of a fixed point is assured for the integral application defined by:

$$u(x) = W[u(x)] \quad (11)$$

with $W(u)$ defined by (8).

Naturally the fixed point of the application (11) will be also the solution of the BVP (1) - (3) under analysis.

So that, using the application (11), with F a function with Lipschitz constant L which verifies (10), an infinite sequence of real functions $u_n = u_n(x)$, n = 1, 2, ... can be obtained, with the convergence property given as:

$$\lim_{n\to\infty} u_n(x) = u(x), \forall x \in [0,1] \quad (12)$$

where u is solution of BVP (1) - (3).

III. Analytical Formulation as Power – Series Expression for Solution of BVP (1)-(3)

As case study, a diffusión–reaction phenomena for which the kinetic law $F = F(u)$ is given as:

$$F(u) = (1-u)^{m+p} \cdot exp\left(\frac{cu}{1+du} \right) \quad (13)$$

where the parameters m, p are non-negative integer numbers which denote reaction order, is considered.

The parameter c is given by:

$$c = \gamma \cdot d \quad (14)$$

with γ being the Arrhenius group, that is

$$\gamma = \frac{E}{RT_s}, 2 \le \gamma \le 20 \quad (15)$$

E is the activation energy, R the universal gases constant and T_s the surfacial temperature of the catalytic particle.

The parameter d denotes the thermicity of the reaction, being $d < 0$ and $d > 0$ respectively for endothermic and exothermic chemical reaction. In what follows, the following general restrictions on the parameters are considered:

$$\begin{aligned} &m, p = 0,1,2,...;\ -1 < d < 1;\ 0.1 \le \phi \le 4; \\ &-20 \le c \le 20 \end{aligned} \quad (16)$$

The Table I below shows values of constant L for the function F given by (9), corresponding to different sets of values for parameters, in the context of the general restriction (16).

TABLE I
VALUES OF CONSTANT L FOR THE FUNCTION F GIVEN BY (9)

Case	*Parametric set*	L
1º	$m = 0,\ p = 0,\ d < 0,\ c < 0$	$-c$
2º	$m = 1,\ p = 0,\ -\frac{1}{2} \le d < 0,\ c < 0$	$\lvert c - 1 \rvert$
3º	$m=1,\ p=0,\ 0 < \lvert d \rvert < 1,\ c > 0$	$exp\left[\frac{c}{1+d}\right]$
4º	$m = 2,\ p = 0,\ d < 0,\ c < 0$	$\lvert c - 2 \rvert$

Inserting (13) in (1), the following particular BVP is obtained:

$$\frac{d^2u}{dx^2} = -\phi^2 (1-u)^{m+p} \cdot exp\left(\frac{cu}{1+du}\right) \; for \; 0 < x < 1 \quad (17)$$

$$u = 0 \; at \; x = 0 \quad (18)$$

$$\frac{du}{dx} = 0 \; at \; x = 1 \quad (19)$$

Now, notice that in view of (13), assumption (**H$_0$**) holds and consequently the integral representation given by (5) can be written as:

$$\begin{aligned} u(x) = m_0 x - \frac{\phi^2}{2} x^2 + \\ -\phi^2 \int_0^x \left\{ \int_0^t \left[c - (m+p) \right] u(z)\, dz \right\} dt + \\ -\phi^2 \int_0^x \left\{ \int_0^t \left[\sum_{k=2}^{\infty} C_k u^k(z) \right] dz \right\} dt \end{aligned} \quad (20)$$

where C_k denotes the corresponding Mac Laurin coefficients for the function F given by (13). For example it results:

$$c_2 = \frac{1}{2} \phi^2 \left[(m+p)(m+p-1-2c) + 2cd - c \right] \quad (21)$$

Now, it is claimed that the integral representation (11) reveals the existence of an analytical formulae with a power-series structure for the solution u of the BVP (17)-(19). In fact, let $u_0 \equiv 0$ be proposed as the zero order approximation in (11) (notice that u_0 verifies the boundary condition (18)). Then, approximations of first an second order u_1 and u_2 from (11) follow as:

$$u_1(x) = m_0 x - \frac{\phi^2}{2} x^2 \quad (22)$$

$$\begin{aligned} u_2(x) = m_0 x - \frac{\phi^2}{2} x^2 - \phi^2 \frac{m_0}{6} \left[c - (m+p) \right] x^3 + \\ -\phi^2 \int_0^x \left\{ \int_0^t \left[\sum_{k=2}^{\infty} C_k \left(m_0 z - \frac{\phi^2}{2} z^2 \right)^k dz \right] \right\} dt \end{aligned} \quad (23)$$

and so on, the following successive approximations $u_3(x), u_4(x), \ldots u_n(x), \ldots$.

Already from (23) it is clear that the contractive integral application introduced by (11) lead to a convergent power-series to represent the function $u = u(x)$ solution of the BVP (17) - (19), that is:

$$\lim_{n \to \infty} u_n(x) = u(x), \; x \in (0,1) \quad (24)$$

with u in (24) given as:

$$u = \sum_{k=0}^{\infty} D(k) x^k, \; x \in (0,1) \quad (25)$$

where D_k can be obtained following a systematic procedure reported in [8], where a power serie expression like (25) was assumed a priori as solution of a BVP like (17) – (19).

In such paper, the following relation to obtain D_k was provided:

$$D(k+2) = -\frac{\phi^2 U_k}{(k+1)(k+2)}, \; \forall_k = 0,1.... \quad (26)$$

From (26) result:

$$D(2) = -\frac{\phi^2}{2} U_0 \quad (27)$$

U_k can be obtained from the following expression, reported also in [8]:

$$U_k = \sum_{r=0}^{k} G_r E_{k-r} \quad (28)$$

being G_k and E_k given as:

$$G_k = \sum_{r=0}^{k} B_r C_{k-r}, \; E_k = \sum_{r=0}^{\infty} d_r \; A_{r(k)} \quad (29)$$

such as it can be seen in [8], where also the procedure to obtain the coefficients $B_r C_{k-r}$, and d_r, was reported. Then, applying the preceding relations result:

$$D(3) = -\frac{\phi^2}{6} U_1, \; U_1 = G_0 E_1 + G_1 E_0 \quad (30)$$

$$U_0 = G_0 E_0, \; E_0 = 1, \; G_0 = 1, \; E_1 = m_0 c \quad (31)$$

$$U_1 = m_0 \left[c - (m+p) \right], \; G_1 = -p m_0 - m m_0 \quad (32)$$

and consequently:

$$D(2) = -\frac{\phi^2}{2}, \; D(3) = -\frac{\phi^2}{6} m_0 \left[c - (m+p) \right] \quad (33)$$

and so on $D(4), \ldots$

In virtue of the boundary conditions (18) and (19), it is obtained:

$$D(0) = 0, D(1) = m_0 \quad (34)$$

Then, inserting (33) and (34) in (25) it gives:

$$u = m_0 x - \frac{\phi^2}{2} x^2 - \frac{\phi^2}{6} m_0 \left[c - \left(m + p \right) \right] x^3 + \\ + \sum_{k=4}^{\infty} D(k) x^k \tag{35}$$

Notice that (23) and (35) contain exactly the same terms up to power x^3.

IV. Numerical Results

Below, the solution u and its derivative for the BVP (17) – (19) are depicted for several sets of values of parameters, and illustrated also with the corresponding graphical representations. Such solution was obtained by applying a power-series expression provided in [8], where the first two cases (as well as many other) are depicted. All those cases show a very good agreement with values taken there for comparison purpose.

Now another cases, where it can be observed that the power-series converges even with $L > \frac{2}{\phi^2}$, are reported. Notice that such bound can be improved to $L < \frac{\pi^2}{2} \frac{1}{\phi^2} = \frac{4.9348}{\phi^2}$ =Upbound, using a result on uniqueness of solution reported in [9].

TABLE II
CASE 1: m = 2 p = 0 c = -0.5 d = -0.1 ϕ = 0.8
$L = |c\text{-}2| = 2.5 < \frac{2}{\phi^2} = 3.125$

x	u(x)	u'(x)
0	0	0.4479408496
0.1	0.04170733854	0.3872792423
0.2	0.07764882875	0.3324161207
0.3	0.1083461628	0.2822277919
0.4	0.134219448	0.2357963956
0.5	0.1556051044	0.1923587122
0.6	0.1727693178	0.1512677118
0.7	0.1859181196	0.1119629901
0.8	0.1952048386	0.07394741343
0.9	0.2007354454	0.03676805679
1	0.2025721451	2.997454930E-17

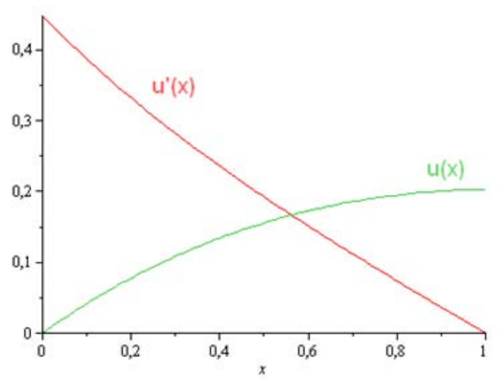

Fig. 1. Graphical representations of case 1

TABLE III
CASE 2: m = 2 p = 0 c = -0.5 d = -0.1 ϕ = 0.5
$L = |c\text{-}2| = 2.5 < \frac{2}{\phi^2} = 8.0$

x	u(x)	u'(x)
0	0	0.2104805726
0.1	0.01981916034	0.1861056446
0.2	0.03725867213	0.1628577125
0.3	0.05242259825	0.1405672154
0.4	0.06539893726	0.119081846
0.5	0.07626118366	0.09826333792
0.6	0.0850695915	0.07798472613
0.7	0.09187218335	0.05812797563
0.8	0.09670553667	0.03858189102
0.9	0.09959537229	0.01924023572
1	0.1005569627	-2.04477392E-15

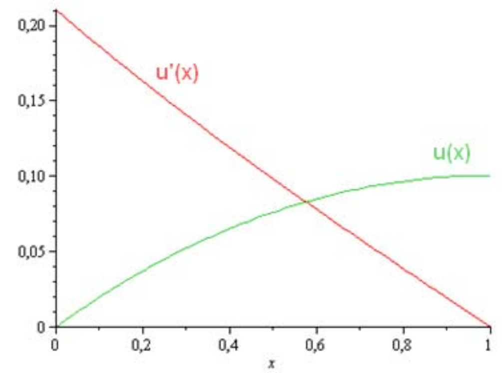

Fig. 2. Graphical representations of case 2

TABLE IV
CASE 3: m = 1 p = 0 c = -0.5 d = -0.1 ϕ = 1.5
$L = |c\text{-}1| = 1.5 > \frac{2}{\phi^2}$ =0.888, BUT 1.5< $\frac{4.9348}{\phi^2}$ = 2.1932

x	u(x)	u'(x)
0	0	1.235876642
0.1	0.112987671	1.029952587
0.2	0.2070553249	0.8560579087
0.3	0.2850186057	0.7068023688
0.4	0.3490490071	0.5765839978
0.5	0.4008238605	0.461048171
0.6	0.4416315325	0.3567195127
0.7	0.4724457195	0.2607438418
0.8	0.4939777431	0.1707010626
0.9	0.5067125148	0.08446079506
1	0.5109297127	-1.47486E-19

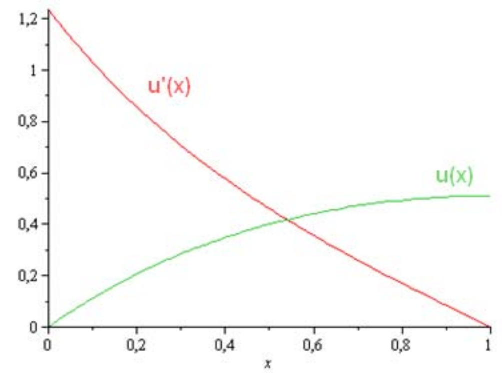

Fig. 3. Graphical representations of case 3

TABLE V

CASE 4: m = 1 p = 0 c = 0.3 d = -0.5 ϕ = 2.1

$$L = exp\left[\frac{c}{1+d}\right] = 1.822 > \frac{2}{\phi^2} = 0.4535, \text{ AND ALSO } L > \frac{4.9348}{\phi^2} = \text{Upbound} = 1.119.$$

(L = 1.628* Upbound, BUT SERIES CONVERGES)

x	u(x)	u'(x)
0	0	2.212167773
0.1	0.2002682193	1.803854478
0.2	0.3627674103	1.455469818
0.3	0.493109809	1.159534116
0.4	0.5961933536	0.9091815939
0.5	0.6762466262	0.6978465464
0.6	0.7368473877	0.5190524498
0.7	0.7809255201	0.366309208
0.8	0.8107601808	0.23309446
0.9	0.8279783805	0.1129088705
1	0.8335787224	-2.541810215E-16

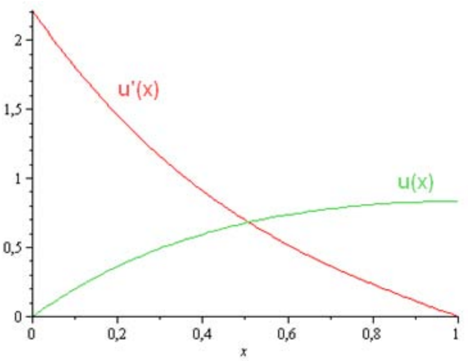

Fig. 4. Graphical representations of case 4

TABLE VI

CASE 5: m = 1 p = 0 c = 1.3 d = -0.5 ϕ = 1.1

$$L = exp\left[\frac{c}{1+d}\right] = 13.46 > \frac{2}{\phi^2} = 1.6529, \text{ AND ALSO } L > \frac{4.9348}{\phi^2} = \text{Upbound} = 4.0783.$$

(L = 3.3* Upbound, BUT SERIES STILL CONVERGES!)

x	u(x)	u'(x)
0	0	1.405446642
0.1	0.134407745	1.281821987
0.2	0.2561820696	1.152737866
0.3	0.3647708267	1.018134125
0.4	0.4596372317	0.8783987717
0.5	0.5403096225	0.7344514435
0.6	0.6064334048	0.5876885935
0.7	0.6578074139	0.4397203128
0.8	0.6943840842	0.2919273788
0.9	0.7162244186	0.1450630141
1	0.7234499401	-5.939497064E-14

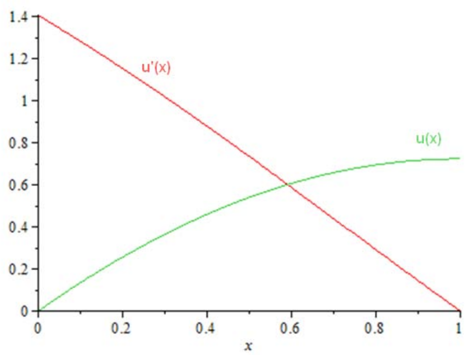

Fig. 5. Graphical representations of case 5

TABLE VII

CASE 6: m = 1 p = 0 c = 1.3 d = -0.5 ϕ = 1.4

$$L = exp\left[\frac{c}{1+d}\right] = 13.46 > \frac{2}{\phi^2} = 1.0204, \text{ AND ALSO}$$

$$L > \frac{4.9348}{\phi^2} = \text{Upbound} = 2.5178.$$

(L=5.346*Upbound. FINALLY, SERIES DOESN'T CONVERGE TO SOLUTION!).

x	u(x)	u'(x)
0	0	1.001999314
0.1	0.09030370445	0.8031358411
0.2	0.1604515787	0.5990185046
0.3	0.2099655164	0.3906554582
0.4	0.2384853358	0.1793792645
0.5	0.2457954937	-0.0332702673
0.6	0.2318398445	-0.2456634623
0.7	0.1967252585	-0.4561871006
0.8	0.1407144909	-0.6633582415
0.9	0.0642051529	-0.8660033166
1	-0.03230046165	-1.062783883

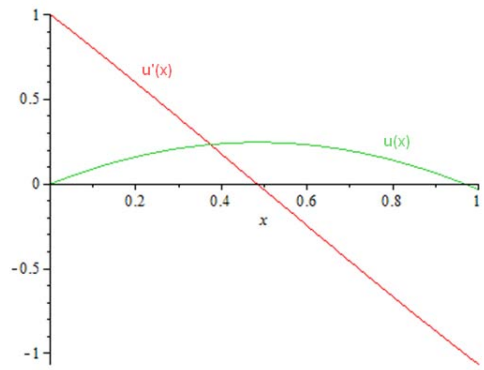

Fig. 6. Graphical representations of case 6

V. Conclusion

The theoretical fundaments which demonstrate the existence and uniqueness of the solution of a typical nonlinear BVP have been presented. The solution was obtained by using the well-known power-series method. An opportune integral operator was introduced.

It must be noted that a wide class of nonlinear kinetic laws can be considered, whenever they belong to the class of Lipschitzian functions with respect to the unknown function in the BVP under analysis.

As it can be seen in some of illustrated cases, power-series resulted to be convergent even when parameters were out of the calculated convergence zone. So, the problem deserves more studies about it. Surely, a greater convergence zone can be obtained by using another norm in the vectorial space V defined in (6).

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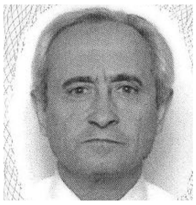

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