2019

Approximate Analytical Solution for Mathematical Models of Thermal Ignition and Non-Isothermal Catalytic Zero Order Reaction in a Spherical Geometry

Moustafa A. Soliman
The British University in Egypt, moustafa.aly@bue.edu.eg

Journal of King Saud University – Engineering Sciences 31 (2019) 164–170

Contents lists available at ScienceDirect

Journal of King Saud University – Engineering Sciences

journal homepage: www.sciencedirect.com

Original article

Approximate analytical solution for mathematical models of thermal ignition and non-isothermal catalytic zero order reaction in a spherical geometry

Moustafa Aly Soliman

Chemical Engineering Department, The British University in Egypt, P.O. Box 43, El Shorouk City, Cairo 11837, Egypt

ARTICLE INFO

Article history:
Received 18 February 2017
Accepted 17 May 2017
Available online 20 May 2017

Keywords:
Lane-Emden equation
Frank-Kamenetskii equation
Spherical annulus
Thermal ignition
Zero order reaction
Catalyst particle
Effectiveness factor

ABSTRACT

In this paper an approximate analytical solution for the Frank-Kamenetskii equation modeling thermal ignition without the depletion of the combustibles in a spherical annulus and non-isothermal zero order reaction in spherical catalyst particle is presented. The approximate solution is compared with the numerical solution and is in good agreement with the numerical solution. The approximate solution obtained is valid for all values of the distance parameter. Multiple solutions occur for some range of Frank-Kamenetskii parameter (λ). The multiplicity is infinite for the case of a solid sphere and $\lambda = 2$. Interesting relation is obtained for λ at the turning points. For the non-isothermal zero order reaction in a spherical catalyst particle the effectiveness factor was obtained using the approximate solution. The values of the effectiveness factor obtained from the approximate solution are accurate compared with the exact values obtained from numerical computations.

1. Introduction

The problems of thermal explosion or ignition of a combustible material in a hollow sphere and zero order reaction in non-isothermal spherical catalyst particle are examined in this paper. The governing equation was derived by Frank-Kamentskii. The steady state equation in an enclosure is given by

$$k\left(\frac{d^2T}{dR^2}+\frac{s}{R}\frac{dT}{dR}\right\} = -(-\Delta H)A\exp\left(\frac{-E}{R_gT}\right) \tag{1}$$

Here, the constant k is the thermal conductivity, $(-\Delta H)$ is the heat of reaction, Arrhenius kinetics is assumed with A the frequency factor, E the energy of activation of the chemical reaction, R_g is the gas constant, and T denotes the absolute temperature. In addition we assumed that consumption of combustible material is neglected, i.e, zero order reaction. R is the spatial variable expressing the distance from the center of the enclosure. s is a shape factor that takes a value of 0 for an infinite slab, 1 for an infinite cylinder and 2 for a sphere.

Introduce the following change of variables;

$$u = \frac{E(T-T_0)}{R_gT_0^2};\varepsilon = \frac{RT_0}{E};r = \frac{R}{a};\lambda = \frac{(-\Delta H)EAa^2}{kR_gT_0^2}\exp\left(\frac{-E}{R_gT_0}\right)$$

to obtain

$$\frac{d^2u}{dr^2}+\frac{s}{r}\frac{du}{dr} = -\lambda\exp\left(\frac{u}{1+\varepsilon u}\right) \tag{2}$$

where a is the radius of the enclosure and T_0 is the ambient absolute temperature.

For small ε (Large activation energy), we can approximate Eq. (2) by

$$\frac{d^2u}{dr^2}+\frac{s}{r}\frac{du}{dr} = -\lambda\exp(u) \tag{3}$$

This equation is the Frank-Kamenetskii equation (Frank-Kamenetskii, 1955). Using $\varepsilon = 0$ in Eq. (2) is called Frank-Kamenetskii approximation and λ is called Frank-Kamenetskii parameter. If λ is greater than a critical value, explosion occurs and there is no solution for the equation. For λ less than the critical

E-mail address: moustafa.aly@bue.edu.eg

Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

http://dx.doi.org/10.1016/j.jksues.2017.05.001
1018-3639/© 2017 The Author. Production and hosting by Elsevier B.V. on behalf of King Saud University.

value, two solutions exist for the case of slab and cylinder. For the case of a sphere for different values of λ we can have no solution, one, two or multiple number of solutions. The solution is characterized by infinite number of solutions at $\lambda = 2$ (Britz et al., 2011).

The appropriate boundary conditions in this case are

$$u(1) = 0 \tag{4}$$

$$\frac{du}{dr}|_{r=r_0} = 0 \tag{5}$$

where r_o is the dimensionless inside radius for a hollow enclosure.

Several theoretical studies and numerical methods were used for the study of the Frank-Kamenetskii equation (Adler, 2011; Aris, 1975; Britz et al., 2011; Chandrasekhar, 1967; Enig, 1967; Frank-Kamenetskii, 1955; Hlavacek and Marek, 1968; Hermann and Saravi, 2016; Steggerda, 1965) which models thermal explosion in an enclosure. The equation also models a non-isothermal zero order reaction in a catalyst particle. Frank-Kamenetskii (1955) formulated the problem and obtained analytical solutions for the case of a slab and cylinder enclosure. The spherical enclosure case can so far only be obtained numerically or approximately using perturbation methods. Results for the case of sphere can be found in references (Iacono and De Felice, 2014; Nouh, 2004; Raga et al., 2013; Roger and Van Gorder, 2013; Soliman and Al-Zeghayer, 2015, Van Gorder, 2011). The case of spherical annulus is treated in references (Gill et al., 1979; Hlavacek and Marek, 1968; Wake and Hood, 1993; Hood and Wake, 1996; Soliman, 2019). Numerical methods that can be used to solve Frank-Kamenetskii equation include finite difference, finite elements, collocation methods (Alhumaizi and Soliman, 2000; Finlayson, 1980; Soliman and Alhumaizi, 2008, 2005), and Pade approximants (Khader, 2013, Soliman, 2013, 2017).

The Frank-Kamenetskii equation can be transformed to initial value problem known as Lane-Emden equation of the second kind or isothermal Lane-Emden equation.

Let;

$$\psi = u_0 - u \tag{6}$$

and

$$\xi^2 = \lambda r^2 z^2 \tag{7}$$

where

$$u_0 = u(r_0) \tag{8}$$

$$z^2 = \exp(u_0) \tag{9}$$

Eqs. (3)–(5) become

$$\frac{d^2\psi}{d\xi^2} + \frac{s}{\xi}\frac{d\psi}{d\xi} = \exp(-\psi) \tag{10}$$

$$\psi(\xi_0) = 0 \tag{11}$$

$$\frac{d\psi}{d\xi}|_{\xi=\xi_0} = 0 \tag{12}$$

where ξ_0 is the inner radius of the annulus of the infinite enclosure such that $r_0 = \xi_0 / \xi$.

Eqs. (10)–(12) are the initial value problem analogue to the boundary value problem (3)–(5). Eqs. (10)–(12) are called Lane-Emden equation of the second kind and in spherical enclosure occurs in the theory of stellar structure.

Soliman and Al-Zeghayer (2015) obtained an approximate solution for the Lane-Emden equation in the case of solid sphere. Soliman (2019) extended this solution to the case of hollow sphere.

Eq. (2) can also describe the steady state differential heat balance for catalyst particles in which non-isothermal zero order reaction takes place. Hlavacek and Marek (1968) used the Frank-Kamenetskii approximation (Eq. (3)) and presented the analytical solutions for the cases of solid and hollow slab and cylinder and the numerical solution for the case of sphere (Britz et al., 2011). Aris (1975) devoted a good part of his book to discuss the Lane-Emden equation and Frank-Kamenetskii equation and their relation to each other. Lopes et al. (2009) used perturbation methods to find approximate solution for zero order reaction in a catalyst slab with convection and diffusion. This work can of course be extended to a spherical catalyst particle.

The aim of the present paper is to extend the results of the Lane-Emden equation to the Frank-Kamenetskii equation and give an approximate analytical solution for Eqs. (3)–(5).

Firstly, we treat the case of solid sphere giving the approximate solution of the Lane-Emden equation and the Frank-Kamenetskii equation. Next some useful relations between system parameters for large distance parameter are derived and numerical results are presented. We improve then the approximate solution for the initial value problem (Eqs (8)–(10)) obtained by Soliman (2019) for the case of hollow sphere. We present numerical results to show the accuracy of the equations. The results are extended to the boundary value problem of Frank-Kamenetskii and numerical results are presented. The approximate solution of the effectiveness factor for the model equation is obtained and compared with the exact numerical solution obtained by the solution of the initial value problem.

2. Mathematical development

During mathematical manipulations we will exploit Eqs. (6) and (7) to relate the variables ψ, and ξ of the initial value problem with the variables u, r and the parameter λ of the boundary value problem. Our main concern is the solution of the boundary value problem.

First we introduce previous results in case of solid sphere and then obtain some interesting relations.

2.1. Solid sphere

Soliman and Al-Zeghayer (2015) obtained the following approximate solution for the case of solid sphere ($\xi_0 = 0$) for the Lane-Emden Eqs. (10)–(12),

$$\psi = \ln\left(1 + \frac{\xi^2}{2}\left(1 - \frac{0.59858}{.\sqrt[4]{1+\xi^2/15}}\cos\left(\frac{\sqrt{7}}{4}\ln(1+\xi^2/23.162231)\right)\right)\right) \tag{13}$$

This solution can be extended to the Frank-Kamenetskii Eqs. (3)–(5) using Eqs. (6) and (7) to be,

$$u_0 - u = \ln\left(1 + \frac{\lambda z^2 r^2}{2}\left(1 - \frac{0.59858}{.\sqrt[4]{1 + \lambda z^2 r^2/15}}\cos \times \left(\frac{\sqrt{7}}{4}\ln(1 + \lambda z^2 r^2/23.162231)\right)\right)\right) \tag{14}$$

Taking into consideration that z^2 is given by Eq. (9) and (14) will be implicit in u_0.

Now, If we let

$$A = -0.59858\sqrt[4]{15} = -1.178 \tag{15}$$

$$B = \frac{\pi}{2} - \frac{\sqrt{7}}{4}\ln(23.162231) = -0.507787 \tag{16}$$

Then for large ξ Eq. (13) can be written as

$$\psi = \ln\left(\left(\frac{\xi^2}{2}\right)\varphi\right) \tag{17}$$

where

$$\begin{aligned}\phi &= \left(1 + \frac{A}{\sqrt{\xi}}\sin\left(B + \frac{\sqrt{7}}{2}\ln\xi\right)\right)\\ &= \left(1 - \frac{1.178}{\sqrt{\xi}}\sin\left(-0.507787 + \frac{\sqrt{7}}{2}\ln\xi\right)\right)\end{aligned} \tag{18}$$

By definition (Eqs. (6) and (7)), the value of ψ at r = 1 is

$$\psi = \ln\left(\frac{\xi^2}{\lambda}\right) = u_0 \tag{19}$$

From Eqs. (17) and (19) the condition for λ = 2 is $\varphi = 1$.
$\varphi = 1$ requires

$$\sin\left(-0.507787 + \frac{\sqrt{7}}{2}\ln\xi\right) = 0 \tag{20}$$

Or

$$\left(-0.507787 + \frac{\sqrt{7}}{2}\ln\xi\right) = n\pi \quad (\text{n is an integer}) \tag{21}$$

Giving

$$\xi = \exp\left\{\frac{2}{\sqrt{7}}(0.507787 + n\pi)\right\} = 1.4679(10.74909)^n \tag{22}$$

Enig (1967) has shown that for any shape, the following relation is satisfied at the turning points

$$\frac{d\psi}{d\zeta} = 2 \tag{23}$$

where

$$\zeta = \ln(\xi) \tag{24}$$

The points which satisfy relation (23) require

$$\frac{d}{d\xi}\left[\frac{1}{\sqrt{\xi}}\sin\left(-0.507787 + \frac{\sqrt{7}}{2}\ln\xi\right)\right] = 0 \tag{25}$$

giving

$$\tan\left(-0.507787 + \frac{\sqrt{7}}{2}\ln\xi\right) = \sqrt{7} \tag{26}$$

Or

$$\begin{aligned}\xi &= \exp\{\frac{2}{\sqrt{7}}(0.507787 + n\pi + 1.209429)\}\\ &= 3.6623(10.74909)^n\end{aligned} \tag{27}$$

2.1.1. Important relations for large ξ (large u_0)

In this section we develop relations for the different variables for large ξ for the turning points and for λ = 2.

From Eqs. (7) and (17) and at r = 1, we have

$$\begin{aligned}\lambda &= \frac{\xi^2}{\exp(\psi)} = \frac{2}{\left(1 + \frac{A}{\sqrt{\xi}}\sin\left(B + \frac{\sqrt{7}}{2}\ln\xi\right)\right)}\\ &\cong 2\left(1 - \frac{A}{\sqrt{\xi}}\sin\left(B + \frac{\sqrt{7}}{2}\ln\xi\right)\right)\end{aligned} \tag{28}$$

At the turning points, from Eq. (26) we have

$$\sin\left(B + \frac{\sqrt{7}}{2}\ln\xi\right) = \pm\sqrt{\frac{7}{8}} = \text{constant} \tag{29}$$

Now from Eq. (27), we have the following relations for large ξ and for subsequent turning points i, i + 1, i = 1, 2,...

$$\frac{\xi_{i+1}}{\xi_i} = 10.74909 \tag{30}$$

This means that ($\boldsymbol{\xi_i}$) forms a geometric sequence with a common ratio of 10.74909. We also have from Eq. (19) and for λ close to a value of 2,

$$\psi_{i+1} - \psi_i = u_{0,i+1} - u_{0,i} = 2\ln\frac{\xi_{i+1}}{\xi_i} = 4.74964 \tag{31}$$

This means that ($u_{0,i}$) forms arithmetic sequence with a common difference of 4.74964.

From Eqs. (28) and (30) we have

$$\frac{\lambda_{i+1} - 2}{\lambda_i - 2} = -\sqrt{\frac{\xi_i}{\xi_{i+1}}} = -\sqrt{\frac{1}{10.74909}} = -0.30501 \tag{32}$$

This means that ($\lambda_i - 2$) forms a geometric sequence with a common ratio of -0.30501.

Relation (31) also holds for subsequent points having λ = 2.

We also have from Eqs. (6), (7), (17), (18) for very large ξ the relation

$$u_0 - u \cong \ln\left(\frac{\xi^2}{2}\right) = \ln\left(\frac{\lambda r^2 \exp(u_0)}{2}\right) \tag{33}$$

From this equation, we obtain for $\lambda = 2$,

$$u \cong -\ln\left(\frac{\lambda r^2}{2}\right) \cong -\ln(r^2) \tag{34}$$

Which is approached for (r) close to 1

2.1.2. Approximate solution for the Frank-Kamenetskii Eqs. (3-5).

Now we discuss how to obtain the solution of Eq. (14) which is the approximate solution for the Frank-Kamenetskii Eq. (3-5).

For a given ξ, we can calculate ψ from Eq. (13)

Now, at r = 1 we have from Eq. (4);

$$u(1) = 0,$$

from Eq. (6)

$$u_0 = \psi + u = \psi$$

and from Eq. (7)

$$\lambda = \xi^2\exp(-\psi)$$

Then for any r

$$\xi^2 = \lambda r^2\exp(u_0)$$

For this new ξ, we can calculate a new ψ from Eq. (13), then

$$u(r) = u_0 - \psi$$

Usually, however, we have λ. Thus, we need to solve the nonlinear algebraic Eq. (14) at r = 1 to obtain u_0. Then we use Eq. (14) again to get u at any r.

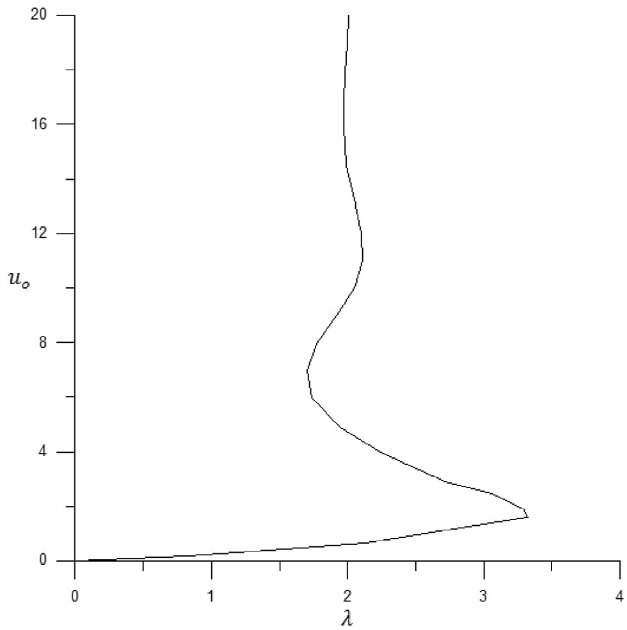

Fig. 1. u_0 against λ.

2.1.2. Numerical results and discussion

We have chosen the DASSL FORTRAN code (Petzold, 1982) to solve Eqs. (10–12). It uses backward differentiation formula method to solve a system of differential algebraic equations.

From the numerical solution we obtained Fig. 1 for a plot of u_0 against λ. The approximate solution is so accurate that it is indistinguishable with the numerical solution. Similar graphical plots are obtained by Britz et al., 2011.

Table 1 shows the values of λ and u_0 for the turning points. The first row contains the values obtained by Steggerda [4]. We notice that the last four values do not satisfy relation (32) and thus they must be in error. The second and third rows are for λ and u_0 calculated from the numerical solution with the last three values predicted from Eqs. (31), (32). We can notice from the last five values the satisfaction of relations (31), (32).

Table 2 shows the values of u_o for λ = 2 calculated from the numerical solution. Again we notice for the last five values the satisfaction of relation (31)

For five significant figures our value for λ (3.32199) for the first turning point is consistent with others (Britz et al., 2011; Steggerda, 1965).

2.2. Hollow sphere

In this section we improve on the approximate solution for Eqs. (8–10) obtained by Soliman (2019).

For this purpose, we define y as

$$y = \xi - \xi_0 \tag{35}$$

and α as

$$\alpha = \frac{\xi_0}{\xi} \tag{36}$$

$$a_1 = \sqrt{\frac{63 * 105}{13}} \tag{37}$$

$$a_2 = \sqrt{\frac{63 * 105}{4}} \tag{38}$$

The approximate solution is given by

$$c\psi_1 = (1-\alpha^q)\ln\left(1+\frac{y^2}{2}\left(1-\frac{2}{3.\sqrt[4]{1+z^2/15}}\cos\left(\frac{\sqrt{7}}{4}\ln(1+u^2/a_1)\right)\right)\right)+ (\alpha-\alpha^q)\ln\left(1+y^2\left(1-\frac{2}{3.\sqrt[4]{1+2z^2/15}}\cos\left(\frac{\sqrt{7}}{4}\ln(1+u^2/a_2)\right)\right)\right) \tag{39}$$

$$\psi_2 = 2\alpha^q \ln\left(\cosh(\frac{y}{\sqrt{2}})\right) \tag{40}$$

$$\psi = \psi_1 + \psi_2 \tag{41}$$

$$z = \frac{y}{(1+\alpha^2 y^2/2)^{n_1}}$$

$$u = \frac{y}{(1+\alpha^2 y^2/2)^{n_2}} \tag{42}$$

Using extensive numerical computations, we arrived at the following values for the parameters q, n_1, and n_2.

$$q = 1 + \frac{2 + 384\alpha y^2/\xi_0^7}{\xi_0(1+3\alpha y^2/\xi_0^7)} \tag{43}$$

$$n_1 = 2.667 + 0.14\xi_0 + 0.00135\xi_0^2 \tag{44}$$

$$n_2 = 4.262(1-\exp(-0.025+0.09\xi_0-0.024\xi_0^2)) \tag{45}$$

To test the accuracy of Eqs. (39–45), Figs. 2–4 are presented as a plot of ψ against λ for the cases of ξ_0 = 5, 20, and 50. We notice that for large ξ_0 and ψ the profile approaches that of a solid sphere with the infinite oscillations around $\lambda = 2$.

Table 1
λ and u_0 for the turning points. * means predicted values.

λ	3.32199	1.66411	2.10834	1.96657	2.0095	1.99571	2.00023	1.99922	
λ	3.32199	1.66416	2.10854	1.96746	2.00998	1.99696	2.00093*	1.99972*	2.00009*
u_o	1.60746	6.74080	11.3768	16.1614	20.9004	25.6532	30.4004*	35.1507*	39.9001*

Table 2
u_0 for λ = 2. * means predicted values.

u_o	0.45698	4.6665	9.61872	14.311	19.0786	23.8228	28.5724*	33.322*	38.0717*

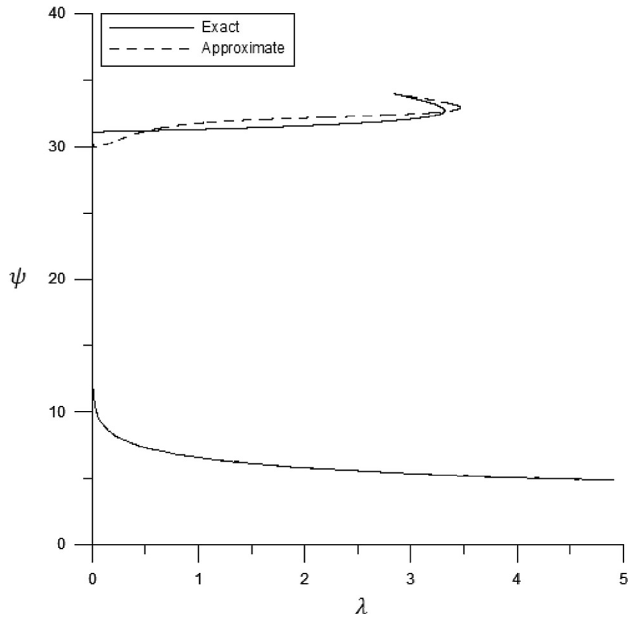

Fig. 2. ψ against λ for ξ_0 = 50.

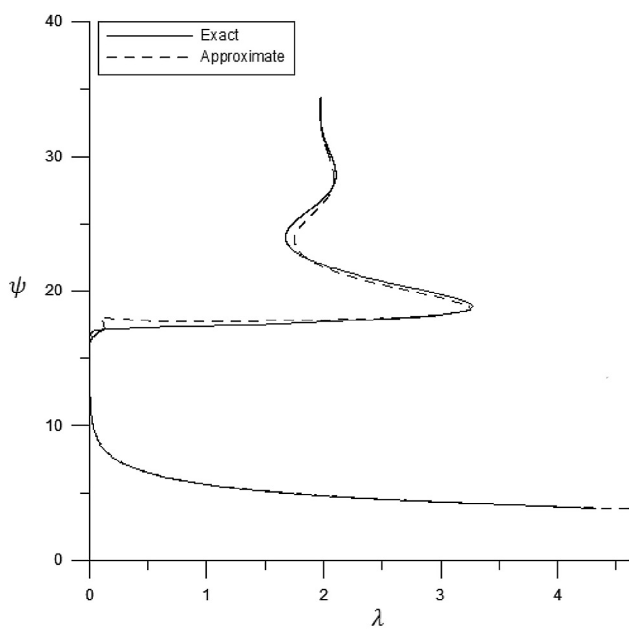

Fig. 3. ψ against λ for ξ_0 = 20.

In general good agreement of the profiles of the approximate solution and the numerical solution is observed.

2.2.1. Approximate solution for the Frank-Kamenetskii Eqs. (3–5)

Eqs. (39–45) hold for the case of hollow sphere while replacing

$$\xi = \sqrt{\lambda} r \exp(u_0/2) \tag{46}$$

$$\xi_0 = \sqrt{\lambda} r_0 \exp(u_0/2) \tag{47}$$

$$\psi = u_0 - u \tag{48}$$

Given u_0, and r_0, and using the substitutions (46–48), Eqs. (39–45) evaluated at $r = 1$ become a non-linear equation in λ. This non-linear equation is solved for λ for different values of r_0 and the results are plotted in Figs. 5–8.

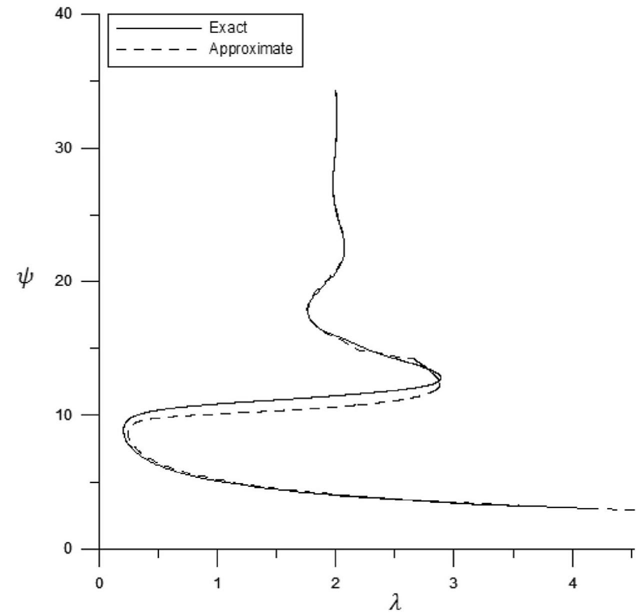

Fig. 4. ψ against λ for ξ_0 = 5.

Figs. 5–8 show a plot of the exact numerical solution and the approximate solution given by Eqs. (39–45) of u_0 against λ for a certain value of r_0. The numerical solution is obtained by using DASSL (Petzold, 1982) for the solution of the Lane-Emden Eqs. (10–12) for different values of the annulus radius ξ_0 and recording ψ as u_0 and λ as $\xi^2 e^{-u_0}$ for $\xi = \xi_0/r_0$. The accuracy of the approximate solution is very good especially for $r_0 = 0.8$ (Fig. 5). Some deviations in small range of λ occur in other cases (at the limit point in Fig. 6 and at the middle of Figs. 7, 8 in Figure). The limit point in Fig. 6 is over-estimated by about 6% while the maximum under-estimation of λ is 6% in Fig. 7 and 13% in Fig. 8.

Contrary to the case of a solid sphere, the solution has a finite number of multiplicity. Wake and Hood (1993) showed that there exist at least two solutions, the multiplicity of solutions is finite and the number of solutions increases as r_0 approaches 0. These conclusions are confirmed by the present calculations. Hood and Wake (1996) classified the solution as slab like when it has two solutions (Figs. 5–7), and as sphere like when it shows oscillations around λ = 2 (Fig. 8) before it goes to infinity as λ goes to zero. They estimated that the difference in behavior occurs at r_0 = 0.02969 with slab like behavior for r_0 > 0.02969.

2.3. Effectiveness factor for a zero order reaction in a non-isothermal catalyst particle

2.3.1. Mathematical formulation

In the case of a nonisothermal reaction of zero-order (and also of order between 0 and 1) the concentration of a reactant within the catalyst particle can fall to zero at a certain distance off the centre of the particle.

The temperature reaches a maximum at this point ($r = r_0$) for an exothermic reaction. Thus we have,

$$\frac{du}{dr}\Big|_{r=r_0} = 0$$

and we will have a situation similar to combustion in a spherical annulus.

If the reactant has an initial concentration of C_{A0}, there will be a maximum temperature which could not be exceeded. This temper-

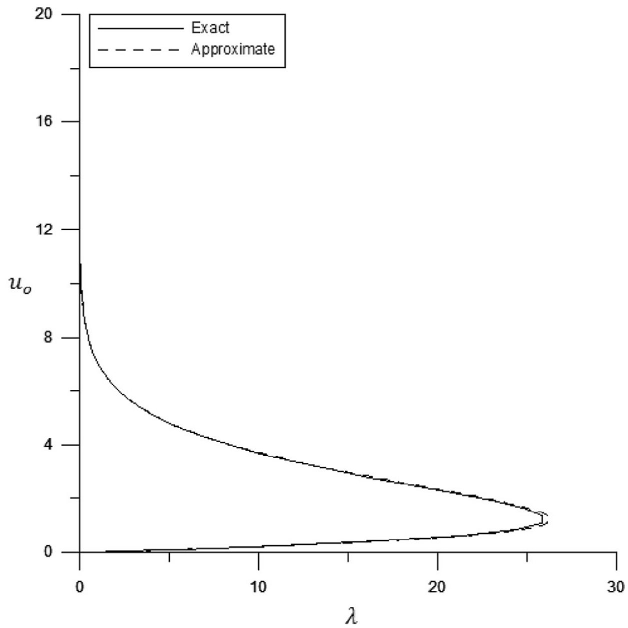

Fig. 5. u_0 against λ for the case of a hollow sphere with $r_0 = 0.8$.

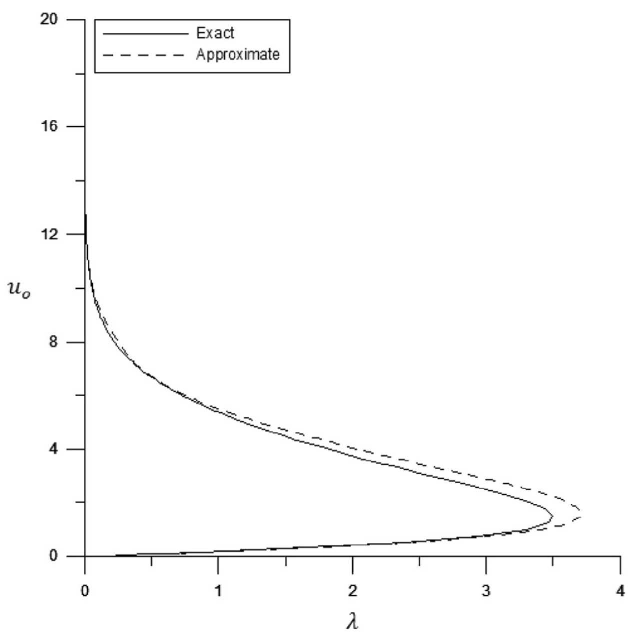

Fig. 6. u_0 against λ for the case of a hollow sphere with $r_0 = 0.2$.

ature corresponds to the disappearance of the reactant and is given by

$$T_{\max} - T_0 = \frac{C_{A0}D(-\Delta H)}{k} \tag{49}$$

To relate the present work with the familiar terminology of diffusion and reaction in catalyst particles, we define

Prater Number = dimensionless adiabatic temperature rise=

$$\beta = \frac{T_{\max} - T_0}{T_0} = \frac{C_{A0}D(-\Delta H)}{kT_0} \tag{50}$$

$$\text{Arrhenius Number} = \text{dimensionless activation energy} = \gamma = \frac{E}{R_g T_0} = \frac{1}{\varepsilon} \tag{51}$$

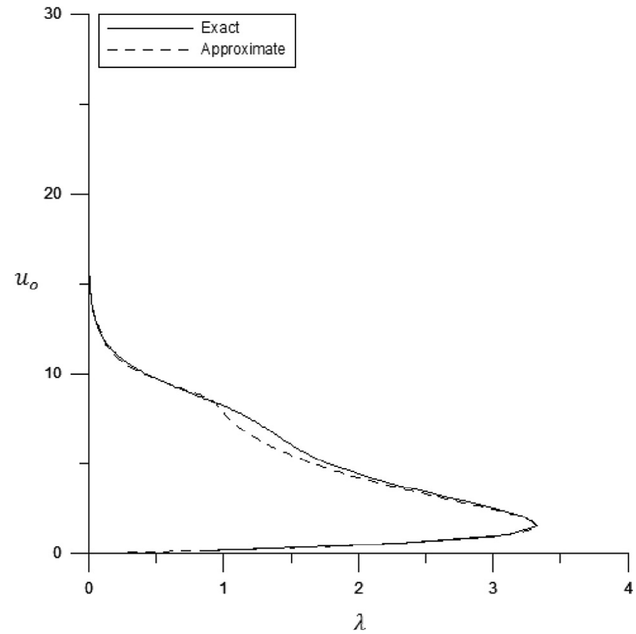

Fig. 7. u_0 against λ for the case of a hollow sphere with $r_0 = 0.05$.

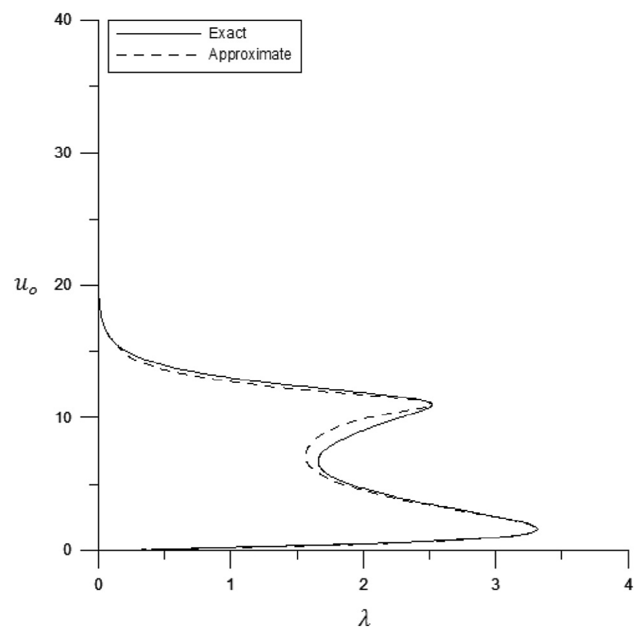

Fig. 8. u_0 against λ for the case of a hollow sphere with $r_0 = 0.01$.

$$\text{Thiele Modulus} = \varphi = a\sqrt{\frac{A\exp(\frac{-E}{R_g T_0})}{DC_{A0}}} = \sqrt{\frac{\lambda}{\beta\gamma}} \tag{52}$$

We can conclude then that

$$u_0 = \beta\gamma \tag{53}$$

$$\lambda = \beta\gamma\varphi^2 \tag{54}$$

The effectiveness factor η is given by

$$\eta = -\frac{3}{\lambda}\frac{du}{dr}\Big|_{r=1} = 3\int_{r_0}^{1} r^2 \exp(u)dr = \frac{3}{\sqrt{\lambda}}\sqrt{2\int_{r_0}^{1} r^4 \exp(u)\frac{du}{dr}dr} \tag{55}$$

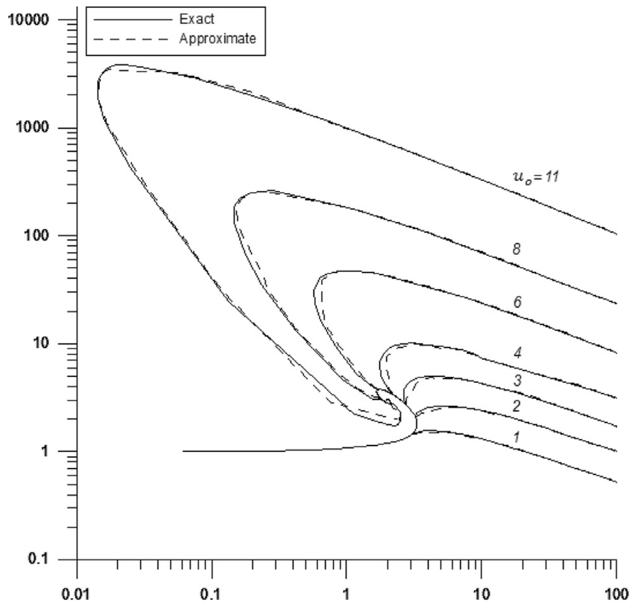

Fig. 9. Effectiveness factor η against λ in a spherical catalyst particle.

The effectiveness factor of a catalyst particle can also be expressed in terms of the solution of the Lane-Emden equation as

$$\eta = \frac{3}{\lambda}[\xi \frac{d\psi}{d\xi}] = \frac{3}{\lambda \xi} \int_{\xi_0}^{\xi} \xi^2 \exp(-\psi) d\xi \quad (56)$$

where

$$\lambda = \xi^2 \exp(-\psi) \quad (57)$$

This means that we can calculate the effectiveness factor directly from the solution of the Lane-Emden equation. Fig. 9 shows the results of these calculations. The exact numerical solution is obtained from $\frac{d\psi}{d\xi}$, while the approximate solution is obtained from the integral formula with ψ calculated from the approximate solution (Eq. (13)). For the main branch which ends at (2,3) the calculations are for solid sphere with $\xi_0 = 0$. For the sub-branches with a given u_0, the equation is solved for different values of ξ_0. The effectiveness factor is the value at $\psi = u_0$. The obtained results are found to be in good agreement with the exact solution. The relative error in the effectiveness factor is less than 10% on the average. The most significant deviations are in the region of maximum value of η. The deviations are insignificant in most of the regions.

3. Conclusions

We presented an approximate analytical solution for the isothermal Lane-Emden Eqs. (39-45) that is valid for all values of distance parameter ξ. The solution is extended to the corresponding Frank-Kamenetskii equation modelling a thermal explosion in a sphere and non-isothermal zero order reaction in a spherical catalyst particle using Eqs. (46–48). As for the actual solution to the boundary value problem, we have seen that the approximate solution is in close agreement with the exact solution. We applied the results of this paper to the calculations of the effectiveness factor of a catalyst particle in which non-isothermal zero order reaction takes place.

References

Adler, J., 2011. The spherical Liouville and associated differential equations. IMA J. Appl. Math. 76, 817–833.
Alhumaizi, K.I., Soliman, M.A., 2000. Studies on the method of orthogonal collocation: V: multiple steady states in catalyst particles. J. King Saud Univ., Eng. Sci. 12 (1), 15–26.
Aris, R., 1975. The Mathematical Theory of Diffusion and Reaction in Permeable Catalyst. Oxford University Press.
Britz, D., Strutwolf, J., Osterby, O., 2011. Digital simulation of thermal reactions. Appl. Math. Comput. 218, 1280–1290.
Chandrasekhar, S., 1967. An Introduction to the Study of Stellar Structure. Dover Publications.
Enig, J.W., 1967. Critical parameters in the Poisson-Boltzmann equation of steady-state thermal explosion theory. Combust. Flame 10, 197–199.
Finlayson, B.F., 1980. Nonlinear Analysis in Chemical Engineering. McGraw-Hill.
Frank-Kamenetskii, D.A., 1955. Diffusion and Heat Exchange in Chemical Kinetics. Princeton University Press.
Gill, W., Donaldson, A.B., Shouman, A.R., 1979. The Frank-Kamenetskii problem revisited. Part I. Boundary conditions of first kind. Combust. Flame 36, 217–232.
Hlavacek, V., Marek, M., 1968. Modelling of chemical reactors – IX the non-isothermal zero-order reaction within a porous catalyst particle. Chem. Eng. Sci. 23, 865–880.
Hermann, M., Saravi, M., 2016. Nonlinear Ordinary Differential Equations: Analytical Approximation and Numerical Methods. Springer.
Hood, M.J., Wake, G.C., 1996. Gelfand's equation in spherical domains: further results and the spherical annulus revisited. Math. Comput. Modell. 24 (8), 47–54.
Iacono, R., De Felice, M., 2014. Approximate analytic solutions to the isothermal Lane-Emden equation. Celest. Mech. Dyn. Astron. 118, 291–298.
Khader, M.M., 2013. On the numerical solutions for chemical kinetics system using Picard-Padé technique. J. King Saud Univ., Eng. Sci. 25 (2), 97–103.
Nouh, M.I., 2004. Accelerated power series solution of polytropic and isothermal gas spheres. New Astron. 9, 467–473.
Lopes, J.P., Cardoso, S.S.S., Rodrigues, A.E., 2009. Convection, diffusion, and exothermic zero-order reaction in a porous catalyst slab: scaling and perturbation analysis. AIChE J. 55 (10), 2686–2699.
Petzold, L.A., 1982. Description of DASSL A differential/algebraic system solver. SAND82-8637.
Raga, A.C., Rodríguez-Ramírez, J.C., Villasante, M., Rodríguez-González, A., Lora, V., 2013. New analytical approximation to the isothermal self gravitating sphere. Rev. Mex. Astron. Astrofis. 49, 63–69.
Reger, K., Van Gorder, R.A., 2013. Lane-Emden equations of second kind modelling thermal explosion in infinite cylinder and sphere. Appl. Math. Mech. 34 (12), 1439–1452.
Soliman, M.A., 2013. Rational approximation for the one-dimensional Bratu equation. Int. J. Eng. Technol. 13 (5), 24–39.
Soliman, M.A., 2017. Rational approximation for Bratu-type equations of solid and hollow geometries. LAP LAMBERT Academic Publishing, Saarbrücken, Germany.
Soliman, M.A., 2019. Approximate solution for the Lane-Emden equation of the second kind in a spherical annulus. J. King Saud Univ. Eng. Sci. 31 (1), 1–5.
Soliman, M.A., Alhumaizi, K., 2005. Studies on the method of orthogonal collocation VI. A moving collocation method for the solution of the transient heat conduction problem. J. King Saud Univ., Eng. Sci. 17, 213–226.
Soliman, M.A., Alhumaizi, K., 2008. Studies on the method of orthogonal collocation VII. An efficient collocation method for diffusion-convection problems with chemical reaction. J. King Saud Univ., Eng. Sci. 20 (2), 95–102.
Soliman, M.A., Al-Zeghayer, Y., 2015. Approximate analytical solution for the isothermal Lane-Emden equation in a spherical geometry. Rev. Mex. Astron. Astrofis. 51, 173–180.
Steggerda, J.J., 1965. Thermal stability: an extension of Frank-Kamenetsky's theory. J. Chem. Phys. 43, 4446–4448.
Van Gorder, R.A., 2011. An elegant perturbation solution for the Lane-Emden equation of the second kind. New Astron. 16, 65–67.
Wake, G.C., Hood, M.J., 1993. Multiplicity of solutions of a Quasilinear elliptic equation in spherical domains. Math. Comput. Modell. 18 (10), 157–162.