Approximations to the Solution of the Frank-Kamenetskii Equation in a Spherical Geometry

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Abstract In this paper, an approximate analytical solution for Frank-Kamenetskii equation modeling a thermal explosion in a sphere, is obtained. The approximate solution is obtained by perturbation methods in terms of small and large distance parameter. The approximate solution is compared with the numerical solution obtained from an initial value problem formulation to the original boundary value problem. The approximate solution obtained is valid for all values of the distance parameter. For the original boundary value problem and for a given Frank-Kamenetskii parameter, a nonlinear algebraic equation needs to be solved to be able to apply the approximate solution.

Keywords Frank-Kamenetskii equation • Thermal explosion • Stellar structure • Perturbation • Sphere

1 Introduction

Several theoretical studies and numerical methods were used for the study of the Frank-Kamenetskii equation [1–12] which models thermal explosion in an enclosure. The equation in a spherical enclosure occurs in the theory of stellar structure. The equation also models a non-isothermal zero order reaction in a catalyst particle. Frank-Kamenetskii [1] formulated the problem and obtained analytical solutions for the case of a slab and cylinder enclosure. More results on the case of a slab and cylinder can be found in references [13–16]. The spherical enclosure case can so far only be obtained numerically.

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The Frank-Kamenetskii equation is given by

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

with the boundary conditions

$$u(1) = 0 \tag{2}$$

$$\frac{du}{dr} |_{r=0} = 0 \tag{3}$$

where 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; u is dimensionless temperature; and r is dimensionless distance.

This equation was treated by different investigators and was thus given different names such as Bratu, Liouville, Gelfand, and Frank-Kamenetskii equation.

The parameter λ is usually given the name of 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 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 $\lambda = 2$.

The aim of the present paper is to give an approximate analytical solution for equations (1–3).

In the next section, we transform the boundary value problem to an initial value problem and obtain approximate solutions for this initial value problem for large and small distance parameter using perturbation methods. Then we modify the solution obtained for large distance parameter to be also valid for the small distance parameter case. Thus we obtain one general approximate solution valid for all values of the distance parameter. Finally numerical results are presented.

2 Mathematical Development

First we change the boundary value problem to an initial value problem as follows:

Let

$$\psi = u_0 - u, u_0 = u(0) \tag{4}$$

and

$$\xi^2 = \lambda r^2 \exp(u_0) \tag{5}$$

Equations (1–3) become

$$\frac{d^2\psi}{d\xi^2} + \frac{s}{\xi}\frac{d\psi}{d\xi} = \exp(-\psi) \tag{6}$$

$$\psi(0) = 0 \tag{7}$$

$$\frac{d\psi}{d\xi} \mid_{\xi=0} = 0 \tag{8}$$

Tables for ψ against ξ for the case of a sphere are given by Chandrasekhar and Wares [16] and Horedt [17].

2.1 Approximate Solution for Large ξ

We treat equation (6) for the case of a sphere (s=2).

We notice that

$$\psi = 2\ln(\xi) - \ln(2) \tag{9}$$

satisfies equation (6) but does not satisfy initial conditions (7, 8). This solution is called singular solution [2]. This solution approaches the exact solution as ξ tends to infinity.

Define

$$\zeta = \ln(\xi) \tag{10}$$

$$\phi = \psi - 2\ln(\xi) + \ln(2) = \psi - 2\zeta + \ln(2) \tag{11}$$

Substituting equation (11) into equation (6), we obtain

$$\frac{d^2\varphi}{d\zeta} + \frac{d\varphi}{d\zeta} + 2 = 2\exp(-\varphi) \tag{12}$$

For small φ (this happens as ξ tends to ∞), we can approximate equation (12) by

$$\frac{d^2\varphi}{d\zeta^2} + \frac{d\varphi}{d\zeta} + 2\varphi = 0 \tag{13}$$

which has a solution in the form

$$\varphi = A\exp\left(-\frac{\zeta}{2}\right)\sin\left(B + \frac{\sqrt{7}}{2}\zeta\right) \tag{14}$$

or

$$\varphi = \frac{A}{\sqrt{\xi}} \sin\left(B + \frac{\sqrt{7}}{2}\ln\xi\right) \tag{15}$$

where A and B are constants to be determined from the numerical solution. φ being small, we can write

$$\varphi = \ln\left(1 + \frac{A}{\sqrt{\xi}} \sin\left(B + \frac{\sqrt{7}}{2}\ln\xi\right)\right) \tag{16}$$

This formula is similar to what was obtained by Chandrasekhar [3] and Adler [9]

Thus from equations (11) and (15), we have

$$\psi = \ln\left(\frac{\xi^2}{2}\right) + \frac{A}{\sqrt{\xi}} \sin\left(B + \frac{\sqrt{7}}{2}\ln\xi\right) \tag{17}$$

We have solved equations (6–8) numerically using DASSL routine [18] and determined the constants A and B. In fact we used the two points $(\xi, \psi) = (210650.464, 23.823), (525665.99, 25.653)$ to obtain A=−1.178, B=−0.507787. The first point corresponds to $\lambda = 2$ at which $\phi = 0$ and the second point to a turning point.

Equation (17) becomes

$$\psi = \ln\left(\frac{\xi^2}{2}\right) - \frac{1.178}{\sqrt{\xi}} \sin\left(-0.507787 + \frac{\sqrt{7}}{2}\ln\xi\right) \tag{18}$$

By definition, the value of ψ at $\lambda = 2$ is

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

so that the condition for $\lambda = 2$ is

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

or

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

giving

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

Enig [8] has shown that for any shape, the following relation is satisfied at the turning points:

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

This means that

$$\frac{d}{d\xi}\left[\frac{1}{\sqrt{\xi}}\sin\left(-0.507787 + \frac{\sqrt{7}}{2}\ln\xi\right)\right] = 0 \tag{24}$$

giving

$$\tan\left(-0.507787 + \frac{\sqrt{7}}{2}\ln\xi\right) = \sqrt{7} \tag{25}$$

or

$$\xi = \exp\left\{\frac{2}{\sqrt{7}}(0.507787 + n\pi + 1.209429)\right\} = 3.6623(10.74909)^n \tag{26}$$

This is the condition for a turning point.

We could repeat the same analysis but defining

$$\zeta = \ln\left(1 + \frac{\xi^2}{2}\right) \tag{27}$$

We arrive at the following formula:

$$\psi = \ln\left(1 + \frac{\xi^2}{2}\right) - \frac{1.178}{\sqrt[4]{2+\xi^2}}\sin\left(-0.507787 + \frac{\sqrt{7}}{4}\ln(2+\xi^2)\right) \tag{28}$$

This formula would extend the range of applicability of equation (18).

We could further improve the accuracy of equation (28) by writing

$$\psi = \ln\left(1 + \frac{\xi^2}{2}\left(1 - \frac{1.178}{\sqrt[4]{2+\xi^2}}\sin\left(-0.507787 + \frac{\sqrt{7}}{4}\ln(2+\xi^2)\right)\right)\right) \tag{29}$$

The condition for $\lambda = 2$ is given by

$$\xi^2 = \exp\left\{\frac{4}{\sqrt{7}}(0.507787 + n\pi)\right\} - 2 \tag{30}$$

and for a turning point is given by

$$\xi^2 = \exp\left\{\frac{4}{\sqrt{7}}(0.507787 + n\pi + 1.209429)\right\} - 2 \tag{31}$$

2.2 Approximate Solution for All ξ

The following formula was synthesized from equation (29)

$$\psi = \ln\left(1 + \frac{\xi^2}{2}\left(1 - \frac{2}{3\sqrt[4]{1+\xi^2/15}}\cos\left(\frac{\sqrt{7}}{4}\ln\left(1+\xi^2/23.162231\right)\right)\right)\right) \tag{32}$$

Notice

$$\exp\left(\frac{4}{\sqrt{7}}\left(0.507787 + \frac{\pi}{2}\right)\right) = 23.162231$$

Equation (32) contains the main components obtained for large ψ and satisfies the small ψ approximation:

$$\psi \cong \frac{1}{6}\xi^2 - \frac{1}{120}\xi^4 \tag{33}$$

For equation (32) to approach equation (29) for large ξ, the constant pre-multiplying the cosine function (2/3) should be 0.59858

since

$$1.178/\sqrt[4]{15} = 0.59858$$

We can then suggest a general formula of the following form:

$$\psi = \ln\left(1 + \frac{\xi^2}{2}\left(1 - \frac{\left(2/3 + 0.59858{*}10^{-6}\xi^6\right)}{(1+10^{-6}\xi^6)\sqrt[4]{1+\xi^2/15}}\cos\left(\frac{\sqrt{7}}{4}\ln\left(1+\xi^2/23.162231\right)\right)\right)\right) \tag{34}$$

3 Numerical Results and Discussion

We have chosen the DASSL FORTAN code [18] to solve equations (6–8). It uses backward differentiation formula method to solve a system of differential algebraic equations. We were able to reproduce the table of Horedt [17] up to a value of $\psi = 14.7$ and go beyond that to a value of 26. Numerical results show that equation (34) is slightly better than equation (32), but both of them are indistinguishable with the numerical solution. To solve the original problem (equations (1–3)) for a given λ we need to solve the nonlinear algebraic equation (5).

4 Conclusions

Approximate analytical solution for the Frank-Kamenetskii equation valid for all values of λ was derived. Numerical solutions of the equation show that the approximate solution is of good accuracy. The Frank-Kamenetskii parameter λ at the turning points has been evaluated to five decimal places. In catalysis, the equation represents an approximation for zero-order reaction in spherical catalyst particle. Future work will be thus to extend the approximate solution to a general order reaction.

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