A note on corrections in approximation of the modified error function

Abstract

This article deals with the evaluation of some integrals involving error-, exponential- and algebraic functions with an objective to derive explicit expressions for the second and third order correction terms in the approximation of the modified error function, playing important role in the study of Stefan problem. The results obtained here appear to be new and resolve the lack of desired monotonicity property in the results presented by Ceretania et al.(1).Results derived here seem to be useful for the researchers working with Stefan problems.

Keywords: Modified error function; Error function; Nonlinear ordinary differential equation; Approximation

1 Introduction

The modified error function was first introduced by Cho and Sunderlard (4) while they were looking for a solution of a Stefen problem, though it was used broadly for solving diffusion problem (5; 6; 7; 8; 9; 10; 11) even before its formal introduction was given by mentioned authors. Initially, the authors in (1) have presented some approximations for the modified error function. The approximate analytical solution of the nonlinear boundary value problem

$$\left[\{1+\delta\ y(x)\}\ y'(x)\right]' + 2\ x\ y'(x) = 1 \tag{1.1}$$

with boundary condition

$$y(0)=0,\ y(\infty)=1 \tag{1.2}$$

was derived by expressing the solution as a power series expansion in powers of the parameter δ present in the equation with coefficients ϕ_n defined on $\mathbb{R}^+$ as

$$\Phi_\delta(x) = \sum_{n=0}^{\infty} \phi_n(x)\delta^n,\quad x>0. \tag{1.3}$$

An approximation $\Psi_{\delta,m}$ of the modified error function $\Phi_\delta(x)$, which is the m-th partial sum, is given by

$$\Psi_{\delta,m}(x) = \sum_{n=0}^{m} \phi_n(x)\delta^n, \; x > 0, \;\; m \in \mathbb{N}_0. \tag{1.4}$$

The authors in (1) obtained first and second order correction $\phi_1(x)$ and $\phi_2(x)$ involved in the approximations $\Psi_{\delta,1}(x)$ and $\Psi_{\delta,2}(x)$ of the modified error function for $\delta > -1$. But it is observed that $\Psi_{\delta,1}(x)$ appears to be better approximation than $\Psi_{\delta,2}(x)$, which is not desirable. The reason could not be addressed completely. Although the two corrections $\phi_0(x)$ and $\phi_1(x)$ was presented as explicit analytical function, the second order correction $\phi_2(x)$ could not be derived explicitly, rather it is obtained in terms of integrals involving products of exponential and error function. The authors suggested that the numerical implementation of the integrals present in $\phi_2(x)$ might introduce non-negligible perturbations. During numerical experiment it is found that the order of magnitude of $\phi_2(x)$ was greater than that of $\phi_1(x)$, which raises uncertainty over the convergence of the series (1.3). To avoid this undesirable property, the authors in this paper have derived explicit expression of $\phi_2(x)$ involving exponential and error function. Furthermore, the explicit expression of the next order correction $\phi_3(x)$ has been obtained by the evaluation of some integrals involving error function and exponential function and by derivation of some recurrence relation, which is not available in the literature yet. With these expressions it is observed that the order of magnitude of the corrections decreases from order to order, which resolves the apparent problem of monotonicity of the successive correction terms that is necessary for the convergence of the series in (1.3). Hence, the inconsonance which arised in (1) can be dispelled.

2 Approximate Solution

Use of expansion (1.4) in Eq.(1.1) with boundary condition (1.2) suggests that the leading order correction $\phi_0(x)$ is solution to the equation [1]

$$\phi_0''(x) + 2\,x\,\phi_0'(x) = 0 \tag{2.1}$$

with

$$\phi_0(0) = 0, \; \phi_0(\infty) = 1. \tag{2.2}$$

The higher order corrections $\phi_n(x)$, $n \in \mathbb{N}$ are solutions to the equation

$$\phi_n''(x) + 2\,x\,\phi_n'(x) = A_{n-1}(x) \tag{2.3}$$

with

$$\phi_n(0) = 0, \; \phi_n(\infty) = 0. \tag{2.4}$$

Here, $A_{n-1}(x)$ is given as

$$A_{n-1}(x) = -\sum_{k=1}^{n} \{\phi_{k-1}'(x)\,\phi_{n-k}'(x) + \phi_{k-1}(x)\,\phi_{n-k}''(x)\}. \tag{2.5}$$

The value of the corrections $\phi_n(x)$ $(n \in \mathbb{N})$ in the expansion (1.3) can be calculated by using two fold integration given as

$$\phi_n(x) = \int_0^x e^{-t^2} \int_0^t e^{s^2} A_{n-1}(s)\, ds\, dt + c_{n,1}\,\text{erf}(x). \tag{2.6}$$

Here, $c_{n,1}$ is the integration constant and erf(x) is error function defined as(3)

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \quad x > 0. \tag{2.7}$$

Now the solution of Eq.(2.1) with boundary condition (2.2) is given by

$$\phi_0(x) = \text{erf}(x). \tag{2.8}$$

With the use of $\phi_0(x)$, we can calculate $A_0(x)$ and $\phi_1(x)$ from (2.5) and (2.6) respectively as

$$A_0(x) = \frac{4\ e^{-x^2}}{\pi}\Big\{\sqrt{\pi}\ x\ \text{erf}(x) - e^{-x^2}\Big\} \tag{2.9}$$

$$\phi_1(x) = \frac{1}{2\pi}\ \Big\{2 - 2\ \sqrt{\pi}\ e^{-x^2} x\ \text{erf}(x) - \pi\ \text{erf}(x)^2 - 2\ e^{-2x^2}\Big\} + c_{1,1}\ \text{erf}(x). \tag{2.10}$$

Using the boundary condition (2.4) we have

$$c_{1,1} = \tfrac{(\pi-2)}{2\pi}. \tag{2.11}$$

Using this value of $c_{1,1}$ in (2.10) one gets

$$\phi_1(x) = \frac{1}{2\pi}\Big[\big\{\pi\ \text{erf}(x) + 2\big\}\ \text{erfc}(x) - 2\ \sqrt{\pi}\ x\ e^{-x^2}\text{erf}(x) - 2\ e^{-2x^2}\Big]. \tag{2.12}$$

Here erfc$(x) = 1 - $ erf(x) is the complimentary error function(3). To obtain the expression for $\phi_2(x)$ we present the following definition and theorems.

Theorem 1. *The integral involving exponential and error function can be represented as*

$$\int_0^x e^{-\lambda y^2}\textit{erf(y)}dy = -2\sqrt{\frac{\pi}{\lambda}}\Big\{T\Big(\sqrt{2}\lambda x, \frac{1}{\sqrt{\lambda}}\Big) - \frac{1}{2\pi}\textit{tan}^{-1}\Big(\frac{1}{\sqrt{\lambda}}\Big)\Big\}. \tag{2.13}$$

Here $T(z,a)$ is Owen T-function defined as(3)

$$T(z,a) = \frac{1}{2\pi}\int_0^a \frac{\textit{exp}\Big\{\dfrac{-z^2(1+t^2)}{2}\Big\}}{(1+t^2)}dt. \tag{2.14}$$

Proof. Differentiating (2.14) w.r.t z and using the transformation $z\ t = \sqrt{2}\ \tau$, we get

$$\begin{aligned}\frac{dT(z,a)}{dz} &= -\frac{1}{2\pi}\int_0^a z\ \text{exp}\Big\{\frac{-z^2(1+t^2)}{2}\Big\}dt \\ &= -\frac{1}{\sqrt{2}\pi}\int_0^{\frac{az}{\sqrt{2}}} \text{exp}\Big(-\frac{z^2}{2}\Big)\ \text{exp}(-\tau^2)\ d\tau \\ &= \frac{-1}{2\sqrt{2}\ \pi}\text{exp}\Big(\frac{-z^2}{2}\Big)\ \text{erf}\Big(\frac{a\ z}{\sqrt{2}}\Big).\end{aligned} \tag{2.15}$$

Further substitution of $a\ z = \sqrt{2}\ y$ followed by integration with respect to y over $[0, x]$ provides

$$\int_0^x \text{exp}\Big(-\frac{y^2}{a^2}\Big)\text{erf}(y)dy = -2\ a\ \sqrt{\pi}\Big\{T\Big(\frac{\sqrt{2}x}{a}, a\Big) - \frac{1}{2\pi}\text{tan}^{-1}(a)\Big\}. \tag{2.16}$$

Choice of $a^2 = \dfrac{1}{\lambda}$ gives the result presented in the statement of the theorem. □

Lemma 1.

$$T(z,1) = \frac{1}{8}\Big\{1 - \text{erf}(\frac{x}{\sqrt{2}})^2\Big\}.$$

Proof. We use the following property of Owen T-function (2)

$$T(z,1) = \frac{1}{2}\, G(z)\big(1 - G(z)\big) \tag{2.17}$$

where $G(z) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{z} e^{-\frac{t^2}{2}}\, dt$.
Now the substitution $\frac{t}{\sqrt{2}} = t'$ converts $G(z)$ into the following form.

$$\begin{aligned} G(z) &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\frac{z}{\sqrt{2}}} e^{-t'^2} dt' \\ &= \frac{1}{\sqrt{\pi}} \left[\int_{-\infty}^{0} e^{-t'^2} dt' + \int_{0}^{\frac{z}{\sqrt{2}}} e^{-t'^2} dt' \right] \\ &= \frac{1}{2} \left[1 + \text{erf}\Big(\frac{z}{\sqrt{2}}\Big) \right] \end{aligned}$$

Substituting the value of $G(z)$ in (2.17) one can obtain the relation stated in the lemma. □

Lemma 2.

$$\int_0^x e^{-x^2} \text{erf}(x) dx = \frac{\sqrt{\pi}}{4} \text{erf}(x)^2.$$

Proof. For $\lambda = 1$ in *Theorem 1* we have

$$\int_0^x e^{-x^2} \text{erf}(x) dx \quad = \quad -2\sqrt{\pi} \Big\{ T(\sqrt{2}x, 1) - \frac{1}{2\pi} \tan^{-1}(1) \Big\}.$$

Using the result obtained in Lemma 1 the statement in this lemma can be proved. □

Definition 1. We define the notation $I_{m,n,\lambda}(x)$ as follows

$$I_{m,n,\lambda}(x) = \int_0^x e^{-\lambda t^2} t^n \text{erf}(t)^m dt. \tag{2.18}$$

Lemma 3. From *Definition-1* it can be observed that

$$\int_0^x e^{-\lambda t^2} t^n \text{erf}(bt)^m dt = \frac{1}{b^{n+1}}\, I_{m,n,\frac{\lambda}{b^2}}(bx) \tag{2.19}$$

where $b \in \mathbb{R}$ is constant.

Proof. Substitution of $bt = t'$ in the integral mentioned in the Lemma converts it into

$$\begin{aligned} & \frac{1}{b^{n+1}} \int_0^{bx} e^{-\frac{\lambda t'^2}{b^2}} t'^n \text{erf}(t')^m \, dt' \\ = \;& \frac{1}{b^{n+1}}\, I_{m,n,\frac{\lambda}{b^2}}(bx). \end{aligned}$$

□

Theorem 2. *The integral $I_{m,n,\lambda}(x)$ given in (2.18) satisfies the recurrence relation*

$$I_{m,n,\lambda}(x) = -\frac{1}{2\lambda} e^{-\lambda x^2} x^{n-1} \textit{erf}(x)^m + \frac{n-1}{2\lambda} I_{m,n-2,\lambda}(x) + \frac{m}{\lambda\sqrt{\pi}} I_{m-1,n-1,\lambda+1}(x) \tag{2.20}$$

where $\lambda > 0$, $m \geq 0$, $n \geq 1$. *It may be observed that*

$$I_{0,0,\lambda}(x) = \frac{\sqrt{\pi}}{2}\ \textit{erf}(x) \tag{2.21}$$

$$I_{0,1,\lambda}(x) = -\frac{1}{2\lambda}\left(e^{-\lambda x^2} - 1\right) \tag{2.22}$$

$$I_{1,0,\lambda}(x) = -2\sqrt{\frac{\pi}{\lambda}}\left\{T\left(\sqrt{2}\lambda x, \frac{1}{\sqrt{\lambda}}\right) - \frac{1}{2\pi}\textit{tan}^{-1}\left(\frac{1}{\sqrt{\lambda}}\right)\right\} \tag{2.23}$$

$$I_{m,0,1}(x) = \frac{\sqrt{\pi}}{2(m+1)}\ \textit{erf}(x)^{(m+1)}. \tag{2.24}$$

Proof.

$$\begin{aligned}
I_{m,n,\lambda}(x) &= \int_0^x e^{-\lambda t^2} t^n \text{erf}(t)^m dt \\
&= -\frac{1}{2\lambda}\int_0^x \frac{d}{dt}\left(e^{-\lambda t^2}\right) t^{n-1}\text{erf}(t)^m dt \\
&= -\frac{1}{2\lambda}\left[t^{n-1}\text{erf}(t)^m \int \frac{d}{dt} e^{-\lambda t^2} dt\right]_0^x + \frac{1}{2\lambda}\left[\int_0^x \frac{d}{dt}\left(t^{n-1}\text{erf(t)}^m\right)\int \frac{d}{dt}(e^{-\lambda t^2}) dt dt\right] \\
&= -\frac{1}{2\lambda}e^{-\lambda x^2} x^{n-1}\text{erf}(x)^m + \frac{n-1}{2\lambda}\int_0^x e^{-\lambda t^2} t^{n-2}\text{erf}(t)^m dt \\
&\quad + \frac{m}{\lambda\sqrt{\pi}}\int_0^x e^{-(\lambda+1)t^2} t^{n-1}\text{erf(t)}^{m-1} dt \\
&= -\frac{1}{2\lambda}e^{-\lambda x^2} x^{n-1}\text{erf}(x)^m + \frac{n-1}{2\lambda} I_{m,n-2,\lambda}(x) + \frac{m}{\lambda\sqrt{\pi}} I_{m-1,n-1,\lambda+1}(x).
\end{aligned}$$

Results in (2.21), (2.22) are obtained by straightforward integration using the *Definition-1* while the result in (2.23) can be established by using *Theorem-1*.
Now,

$$\begin{aligned}
I_{m,0,1}(x) &= \int_0^x \text{erf}(t)^m e^{-t^2}\ dt \\
&= \frac{\sqrt{\pi}}{2(m+1)}\int_0^x \frac{d}{dt}\left(\text{erf}(t)^{m+1}\right)\ dt \\
&= \frac{\sqrt{\pi}}{2(m+1)}\ \text{erf}(x)^{m+1}.
\end{aligned}$$

This completes the proof. □

Theorem 3. *Using Definition-1 we have the following recurrence relation for* $\lambda = 0$

$$I_{m,n,0}(x) = \frac{x^{n+1}}{n+1}\ \textit{erf}(x)^m - \frac{2m}{\sqrt{\pi}(n+1)} I_{m-1,n+1,1}(x). \tag{2.25}$$

Proof. We use the formula for integration by parts to get

$$\begin{aligned}
I_{m,n,0}(x) &= \int_0^x t^n \text{erf}(t)^m\ dt \\
&= \frac{t^{n+1}}{n+1}\ \text{erf}(t)^m\Big|_0^x - \frac{2m}{\sqrt{\pi}(n+1)}\int_0^x \text{erf}(t)^{m-1}\ e^{-t^2} t^{n+1} dt \\
&= \frac{x^{n+1}}{n+1}\ \text{erf}(x)^m - \frac{2m}{\sqrt{\pi}(n+1)} I_{m-1,n+1,1}(x).
\end{aligned}$$

□

Theorem 4. *The explicit expression for the second order correction $\phi_2(x)$ in the approximation of modefied error function $\Phi_\delta(x)$ can be obtained as*

$$\begin{aligned}\phi_2(x) \quad = \quad & \tfrac{1}{4\pi^2}\Big[-2\,\pi\,\mathit{erf}(x)^2\Big\{\pi\,\mathit{erfc}(x)-2\Big\}-4\,e^{-2x^2}\Big\{\pi\left(x^2-3\right)\mathit{erf}(x)+\pi-2\Big\}\\ & +\sqrt{\pi}\,e^{-x^2}x\Big\{\mathit{erf}(x)\{\pi\big(9-2x^2\big)\mathit{erf}(x)-4\pi+8\}-4\Big\}\\ & +\Big\{\pi\left(3\sqrt{3}-8\right)+8\Big\}\mathit{erf}(x)-3\sqrt{3}\,\pi\,\mathit{erf}\left(\sqrt{3}x\right)-2\sqrt{\pi}e^{-3x^2}x+4\pi-8\Big].\end{aligned} \tag{2.26}$$

Proof. From (2.5) one can get,

$$A_1(x) \quad = \quad -\Big\{2\,\phi_0'(x)\,\phi_1'(x)+\phi_1(x)\,\phi_0''(x)+\phi_0(x)\,\phi_1''(x)\Big\} \tag{2.27}$$

Explicit expressions for $\phi_0(x)$, $\phi_1(x)$ given in (2.8) and (2.12) have been used to obtained

$$\begin{aligned}A_1(x) \quad = \quad & \tfrac{4\,e^{-3x^2}}{\pi^2}\Big[-e^{x^2}\left\{2\pi\left(x^2-2\right)\mathrm{erf}(x)+\pi-2\right\}\\ & +\sqrt{\pi}e^{2x^2}x\Big\{\mathrm{erf}(x)\{\pi(x^2-3)\mathrm{erf}(x)+\pi-2\}+1\Big\}-3\sqrt{\pi}x\Big].\end{aligned} \tag{2.28}$$

Using the integral representation of $\phi_n(x)$ in (2.6) for $n=2$, one can obtain the explicit x-dependence of ϕ_2 with the help of *Lemma-2* and *Theorem-2* as

$$\begin{aligned}\phi_2(x) \quad = \quad & \tfrac{e^{-3x^2}}{4\pi^2}\Big[-4e^{x^2}\Big\{\pi\left(x^2-3\right)\mathrm{erf}(x)+\pi-2\Big\}-2\sqrt{\pi}x\\ & -\sqrt{\pi}e^{2x^2}x\Big\{\pi\left(2x^2-9\right)\mathrm{erf}(x)^2+4(\pi-2)\mathrm{erf}(x)+4\Big\}\\ & +e^{3x^2}\Big\{-2\pi\,\mathrm{erf}(x)^2(\pi\,\mathrm{erfc}(x)-2)-3\sqrt{3}\pi\,\mathrm{erf}\left(\sqrt{3}x\right)+4\pi-8\Big\}\Big]\\ & +c_{2,1}\,\mathrm{erf}(x).\end{aligned} \tag{2.29}$$

Use of the boundary condition (2.4) for $n=2$, properties of error- and complementary error-functions provides the integration constant

$$c_{2,1}=\frac{\left(3\pi\sqrt{3}-8\pi+8\right)}{4\pi^2}. \tag{2.30}$$

Relations in (2.29) and (2.30) simultaneously recover the statement of *Theorem-4*. □

The result obtained here appears to be new.

To derive third order correction term $\phi_3(x)$, we recall (2.5) to obtain

$$A_2(x) \quad = \quad -\Big\{\phi_1'(x)^2+2\phi_0'(x)\phi_2'(x)+\phi_0''(x)\phi_2(x)+\phi_1(x)\phi_1''(x)+\phi_0(x)\phi_2''(x)\Big\}. \tag{2.31}$$

Use of explicit expression for $\phi_i(x),\ i=0,1,2$ into the above expression yields a large expression in x which has been split into five parts as

$$A_2(x)=\sum_{k=1}^{5}\,A_{2,k}(x) \tag{2.32}$$

where

$$A_{2,1}(x)=-\tfrac{e^{-2x^2}}{\pi^2}\left(8x^2+6\sqrt{3}+\pi-28+\tfrac{20}{\pi}\right)-\tfrac{18e^{-3x^2}}{\pi^{5/2}}(\pi-2)x-\tfrac{2}{\pi^2}e^{-4x^2}\left(7x^2+4\right), \tag{2.33}$$

$$A_{2,2}(x) = \Big[\tfrac{e^{-x^2}x}{\pi^{5/2}}\Big\{\pi\left(8x^2+6\sqrt{3}+\pi-36\right)+20\Big\} - \tfrac{12\ e^{-2x^2}}{\pi^2}(\pi-2)\left(x^2-2\right) - \tfrac{2e^{-3x^2}x}{\pi^{3/2}}\left(13x^2-32\right)\Big]\text{erf}(x), \tag{2.34}$$

$$A_{2,3}(x) = \Big[\tfrac{6e^{-x^2}x}{\pi^{3/2}}(\pi-2)\left(x^2-3\right) - \tfrac{e^{-2x^2}}{\pi}\left(10x^4-51x^2+48\right)\Big]\text{erf}(x)^2, \tag{2.35}$$

$$A_{2,4}(x) = \tfrac{e^{-x^2}x}{2\sqrt{\pi}}\left(4x^4-36x^2+59\right)\text{erf}(x)^3, \tag{2.36}$$

$$A_{2,5}(x) = -\tfrac{3e^{-x^2}x}{\pi^{5/2}}\Big\{\sqrt{3}\,\pi\ \text{erf}\left(\sqrt{3}x\right)-2\pi+4\Big\}. \tag{2.37}$$

Accordingly, we write $\phi_3(x)$ as

$$\phi_3(x) = \sum_{k=1}^{5}\phi_{3,k}(x) + c_{3,1}\ \text{erf(x)} \tag{2.38}$$

where

$$\phi_{3,k}(x) = \int_0^x e^{-t^2}\int_0^t e^{s^2}A_{2,k}(s)\ ds\ dt. \tag{2.39}$$

Using *Definition-1* and the values of $A_{2,k}(x),\ k=1,2,...,5$ given in (2.33)-(2.37) we can express the integrals $\int_0^t e^{s^2}A_{2,k}(s)\ ds,\ k=1,2,...,5$ as follows.

$$\int_0^t e^{s^2}A_{2,1}(s)\ ds = -\frac{8}{\pi^2}\ I_{0,2,1}(t) - \frac{1}{\pi^2}\Big(6\sqrt{3}+\pi-28+\frac{20}{\pi}\Big)\ I_{0,0,1}(t) - \frac{18}{\pi^{\frac{5}{2}}}(\pi-2)\ I_{0,1,2}(t) - \frac{14}{\pi^2}\ I_{0,2,3}(t) - \frac{8}{\pi^2}\ I_{0,0,3}(t), \tag{2.40}$$

$$\int_0^t e^{s^2}A_{2,2}(s)\ ds = \frac{8}{\pi^{\frac{3}{2}}}\ I_{1,3,0}(t) + \Big(\frac{1}{\pi^{\frac{3}{2}}}(6\sqrt{3}+\pi-36)+\frac{20}{\pi^{\frac{5}{2}}}\Big)\ I_{1,1,0}(t) - \frac{12}{\pi^2}(\pi-2)\ I_{1,2,1}(t) + \frac{24}{\pi^2}(\pi-2)\ I_{1,0,1}(t) - \frac{26}{\pi^{\frac{3}{2}}}\ I_{1,3,2}(t) + \frac{64}{\pi^{\frac{3}{2}}}\ I_{1,1,2}(t), \tag{2.41}$$

$$\int_0^t e^{s^2}A_{2,3}(s)\ ds = \frac{6}{\pi^{\frac{3}{2}}}(\pi-2)\ I_{2,3,0}(t) - \frac{18}{\pi^{\frac{3}{2}}}(\pi-2)\ I_{2,1,0}(t) - \frac{10}{\pi}\ I_{2,4,1}(t) + \frac{51}{\pi}\ I_{2,2,1}(t) - \frac{48}{\pi}\ I_{2,0,1}(t), \tag{2.42}$$

$$\int_0^t e^{s^2}A_{2,4}(s)\ ds = \frac{2}{\sqrt{\pi}}\ I_{3,5,0}(t) - \frac{18}{\sqrt{\pi}}\ I_{3,3,0}(t) + \frac{59}{2\sqrt{\pi}}\ I_{3,1,0}(t), \tag{2.43}$$

$$\int_0^t e^{s^2}A_{2,5}(s)\ ds = \frac{6}{\pi^{\frac{5}{2}}}(\pi-2)\ I_{0,1,0}(t) - \frac{\sqrt{3}}{\pi^{\frac{3}{2}}}\ I_{1,1,0}(\sqrt{3}t). \tag{2.44}$$

We now derive the explicit expressions of $I_{m,n,\lambda}(t)$ for various values of $m,\ n,\ \lambda$ appearing in (2.40)-(2.44) by the use of *Lemma-2, Lemma-3, Theorem-2* and *Theorem-3*. Then using the obtained results and the definition of $\phi_{3,k}(x)$ given in (2.39) one can find the expressions of $\phi_{3,k}(x),\ k=1,2,...,5$ in terms of $I_{m,n,\lambda}(x)$ as

$$\phi_{3,1}(x) = \frac{9}{\pi^{\frac{5}{2}}}\Big(\frac{\pi}{2}-1\Big)I_{0,0,3}(x) + \frac{7}{3\pi^2}I_{0,1,4}(x) + \frac{4}{\pi^2}I_{0,1,2}(x) - \frac{9}{\pi^{\frac{5}{2}}}\Big(\frac{\pi}{2}-1\Big)I_{0,0,1}(x) + \Big(\frac{12}{\pi^{3/2}} - \frac{10}{\pi^{5/2}} - \frac{3\sqrt{3}}{\pi^{3/2}} - \frac{1}{2\sqrt{\pi}}\Big)I_{1,0,1}(x) - \frac{31}{18\pi^{\frac{3}{2}}}I_{1,0,\frac{1}{3}}(\sqrt{3}x), \tag{2.45}$$

$$\begin{aligned}\phi_{3,2}(x) \quad = \quad & \frac{13}{6\pi^2}I_{0,1,4}(x)+\frac{1}{\pi}\Big(\frac{3\sqrt{3}}{\pi}+\frac{1}{2}-\frac{15}{\pi}+\frac{10}{\pi^2}\Big)I_{0,1,2}(x)+\frac{2}{\pi^2}I_{0,3,2}(x)+\frac{6}{\pi}\Big(1-\frac{2}{\pi}\Big)I_{1,1,2}(x)\\ &+\frac{3}{\pi^{3/2}}\Big(1-\frac{2}{\pi}\Big)I_{0,0,3}(x)-\frac{51}{4\pi^{3/2}}I_{1,0,3}(x)+\frac{13}{2\pi^{3/2}}I_{1,2,3}(x)+\frac{3}{\pi^{3/2}}\Big(\frac{2}{\pi}-1\Big)I_{0,0,1}(x)\\ &+\frac{1}{\sqrt{\pi}}\Big(-\frac{3\sqrt{3}}{2\pi}+\frac{15}{2\pi}-\frac{5}{\pi^2}-\frac{1}{4}\Big)I_{1,0,1}(x)+\frac{1}{\sqrt{\pi}}\Big(\frac{10}{\pi^2}+\frac{3\sqrt{3}}{\pi}-\frac{18}{\pi}+\frac{1}{2}\Big)I_{1,2,1}(x)\\ &+\frac{2}{\pi^{3/2}}I_{1,4,1}(x)+\frac{9}{\pi^{3/2}}\Big(\frac{\pi}{2}-1\Big)I_{2,0,1}(x)+\frac{35}{9\pi^{3/2}}I_{1,0,\frac{1}{3}}(\sqrt{3}x), \qquad (2.46)\end{aligned}$$

$$\begin{aligned}\phi_{3,3}(x) \quad = \quad & \frac{5}{3\pi^2}I_{0,1,4}(x)+\frac{12}{\pi^{5/2}}\Big(1-\frac{\pi}{2}\Big)I_{0,0,3}(x)-\frac{3}{\pi^{5/2}}\Big(1-\frac{\pi}{2}\Big)I_{0,2,3}(x)-\frac{31}{2\pi^{3/2}}I_{1,0,3}(x)\\ &+\frac{5}{\pi^{3/2}}I_{1,2,3}(x)+\frac{27}{\pi^2}\Big(1-\frac{\pi}{2}\Big)I_{1,1,2}(x)-\frac{6}{\pi^2}\Big(1-\frac{\pi}{2}\Big)I_{1,3,2}(x)-\frac{18}{\pi}I_{2,1,2}(x)\\ &+\frac{5}{\pi}I_{2,3,2}(x)-\frac{12}{\pi^{5/2}}\Big(1-\frac{\pi}{2}\Big)I_{0,0,1}(x)-\frac{27}{4\pi^{3/2}}\Big(1-\frac{\pi}{2}\Big)I_{2,0,1}(x)\\ &+\frac{18}{\pi^{3/2}}\Big(1-\frac{\pi}{2}\Big)I_{2,2,1}(x)-\frac{3}{\pi^{3/2}}\Big(1-\frac{\pi}{2}\Big)I_{2,4,1}(x)-\frac{5}{\sqrt{\pi}}I_{3,0,1}(x)\\ &+\frac{44}{9\pi^{3/2}}I_{1,0,\frac{1}{3}}(\sqrt{3}x), \qquad (2.47)\end{aligned}$$

$$\begin{aligned}\phi_{3,4}(x) \quad = \quad & -\frac{19}{6\pi^2}I_{0,1,4}(x)+\frac{1}{3\pi^2}I_{0,3,4}(x)+\frac{91}{4\pi^{3/2}}I_{1,0,3}(x)-\frac{10}{\pi^{3/2}}I_{1,2,3}(x)\\ &+\frac{1}{\pi^{3/2}}I_{1,4,3}(x)+\frac{111}{4\pi}I_{2,1,2}(x)-\frac{11}{\pi}I_{2,3,2}(x)+\frac{1}{\pi}I_{2,5,2}(x)\\ &-\frac{37}{8\sqrt{\pi}}I_{3,0,1}(x)+\frac{59}{4\sqrt{\pi}}I_{3,2,1}(x)-\frac{9}{2\sqrt{\pi}}I_{3,4,1}(x)+\frac{1}{3\sqrt{\pi}}I_{3,6,1}(x)\\ &-\frac{127}{18\pi^{3/2}}I_{1,0,\frac{1}{3}}(\sqrt{3}x), \qquad (2.48)\end{aligned}$$

$$\begin{aligned}\phi_{3,5}(x) \quad = \quad & -\frac{3}{2\pi^2}I_{0,1,4}(x)-\frac{6}{\pi^{5/2}}\Big(1-\frac{\pi}{2}\Big)I_{0,2,1}(x)+\frac{1}{4\pi^{3/2}}I_{1,0,\frac{1}{3}}(\sqrt{3}x)\\ &-\frac{1}{2\pi^{3/2}}I_{1,2,\frac{1}{3}}(\sqrt{3}x). \qquad (2.49)\end{aligned}$$

We again derive the expressions for $I_{m,n,\lambda}(x)$ for different $m,\ n,\ \lambda$ present in (2.45)-(2.49) by using *Lemma-2, Lemma-3, Theorem-2* and *Theorem-3* to obtain the explicit expressions for $\phi_{3,k}(x),\ k = 1,2,...,5$ given by

$$\begin{aligned}\phi_{3,1}(x) \quad = \quad & -\frac{1}{216\pi^2}\Big[63\, e^{-4x^2}+216\, e^{-2x^2}-62\sqrt{3}\pi-279+27\Big\{6\pi\left(\sqrt{3}-4\right)+\pi^2+20\Big\}\times\\ &\text{erf}(x)^2+324\,\sqrt{3}\ \text{erf}\left(\sqrt{3}x\right)-162\,\sqrt{3}\ \pi\text{erf}\left(\sqrt{3}x\right)+6\Big\{31\sqrt{3}\ \pi\text{erf}\left(\sqrt{3}x\right)\\ &+81(\pi-2)\Big\}\text{erf}(x)+744\sqrt{3}\pi\ T\left(\sqrt{6}x,\frac{1}{\sqrt{3}}\right)\Big], \qquad (2.50)\end{aligned}$$

$$\begin{aligned}\phi_{3,2}(x) &= \frac{1}{216\pi^3}\Bigg[54\Bigg\{\pi\left(6\sqrt{3}+\pi-28\right)+20+e^{-2x^2}\Bigg\{-\pi\left(4x^2+6\sqrt{3}+\pi-28\right)-20\Bigg\}\\ &-\sqrt{\pi}e^{x^2}x\Bigg\{\pi\left(4x^2+6\sqrt{3}+\pi-30\right)+20\Bigg\}\text{erf}(x)\Bigg\}+54(\pi-2)\pi\times\\ &\Bigg\{-6\left(e^{-2x^2}+1\right)\text{erf}(x)+3\pi\,\text{erf}(x)^3+4\sqrt{3}\,\text{erf}\left(\sqrt{3}x\right)\Bigg\}+\pi\Bigg\{117(1-e^{-4x^2})\\ &-234\sqrt{\pi}e^{-3x^2}x\,\text{erf}(x)+140\sqrt{3}\pi\Bigg\{24\,T\left(\sqrt{6}x,\frac{1}{\sqrt{3}}\right)\\ &+3\,\text{erf}(x)\,\text{erf}\left(\sqrt{3}x\right)-2\Bigg\}\Bigg],\end{aligned} \tag{2.51}$$

$$\begin{aligned}\phi_{3,3}(x) &= \frac{1}{72\pi^{5/2}}\Bigg[27(\pi-2)\Bigg\{\pi e^{-x^2}x\left(9-2x^2\right)\text{erf}(x)^2-4\sqrt{\pi}e^{-2x^2}\left(x^2-4\right)\text{erf}(x)\\ &+8\sqrt{\pi}\,\text{erf}(x)-23\sqrt{\frac{\pi}{3}}\,\text{erf}\left(\sqrt{3}x\right)-2e^{-3x^2}x\Bigg\}+\sqrt{\pi}e^{-4x^2}\Bigg\{-120\sqrt{\pi}e^{x^2}x\,\text{erf}(x)\\ &-45-9\pi e^{2x^2}\left(10x^2-31\right)\text{erf}(x)^2\Bigg\}+\sqrt{\pi}\Bigg\{45-45\pi^2\text{erf}(x)^4\\ &+176\sqrt{3}\pi\Bigg\{12\,T\left(\sqrt{6}x,\frac{1}{\sqrt{3}}\right)+\text{erf}(x)\,\text{erf}\left(\sqrt{3}x\right)-1\Bigg\}\Bigg\}\Bigg],\end{aligned} \tag{2.52}$$

$$\begin{aligned}\phi_{3,4}(x) &= \frac{1}{216\pi^2}\Bigg[e^{-4x^2}(333-36x^2)-54\sqrt{\pi}e^{-3x^2}x\left(2x^2-19\right)\text{erf}(x)\\ &-27\pi e^{-2x^2}\left(4x^4-40x^2+91\right)\text{erf}(x)^2-9\pi^{3/2}e^{-x^2}x\left(4x^4-44x^2+111\right)\text{erf}(x)^3\\ &-\Bigg\{254\pi\sqrt{3}\Bigg\{48\,T\left(\sqrt{6}x,\frac{1}{\sqrt{3}}\right)+3\text{erf}(x)\,\text{erf}\left(\sqrt{3}x\right)-4\Bigg\}+333\Bigg\}\Bigg],\end{aligned} \tag{2.53}$$

$$\begin{aligned}\phi_{3,5}(x) &= \frac{1}{12\pi^{5/2}}\Bigg[9\sqrt{\pi}e^{-4x^2}+9e^{-x^2}x\Bigg\{\sqrt{3}\,\pi\,\text{erf}\left(\sqrt{3}x\right)-2\pi+4\Bigg\}+\sqrt{\pi}\Bigg\{\sqrt{3}\pi-9\\ &-12\sqrt{3}\pi\,T\left(\sqrt{6}x,\frac{1}{\sqrt{3}}\right)-3\text{erf}(x)\Bigg\{\sqrt{3}\,\pi\,\text{erf}\left(\sqrt{3}x\right)-3\pi+6\Bigg\}\Bigg\}\Bigg].\end{aligned} \tag{2.54}$$

Use of (2.50-2.54) in (2.38) and the boundary condition in (2.4) for $n=3$, gives

$$c_{3,1}=\frac{1}{24\pi^3}\left\{(19\sqrt{3}-42)\pi^2+(224-90\sqrt{3})\pi-120\right\}. \tag{2.55}$$

Substituting the derived expressions of $\phi_{3,k}(x),\ k=1,2,...,5$ and the value of $c_{3,1}$ in (2.38) we obtain the explicit expression for the third order correction $\phi_3(x)$ involving error-, complementary error- and

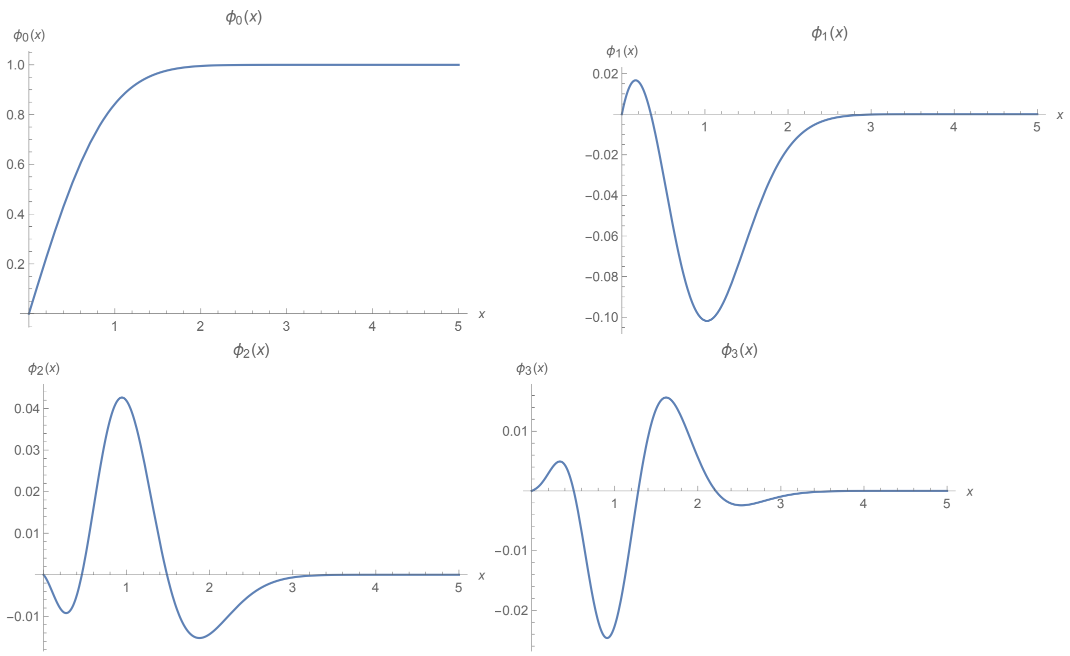

Figure 1: $\phi_n(x)$ for $n = 0, 1, 2, 3$ of Eq.(1.4).

Owen T-functions as

$$
\begin{aligned}
\phi_3(x) \quad = \quad & -\frac{(x^2-5)e^{-4x^2}}{6\pi^2} - \frac{xe^{-3x^2}}{4\pi^{\frac{5}{2}}}\Big\{3(\pi-2)+2\pi(x^2-4)\,\mathrm{erf}(x)\Big\} \\
& -\frac{e^{-2x^2}}{4\pi^3}\Big[20+\pi^2\Big\{1+6(x^2-3)\,\mathrm{erf}(x)+(2x^4-15x^2+30)\,\mathrm{erf}(x)^2\Big\} \\
& +2\pi\Big\{6+3\sqrt{3}-4x^2+6\,(x^2-3)\,\mathrm{erfc}(x)\Big\}\Big] \\
& -\frac{xe^{-x^2}}{24\pi^{\frac{5}{2}}}\Big[6\Big\{20+\pi(4x^2+\pi+6\sqrt{3}-30)\Big\}\,\mathrm{erf}(x)+9\pi(\pi-2)(2x^2-9)\,\mathrm{erf}(x)^2 \\
& +\pi^2\,(4x^4-44x^2+111)\,\mathrm{erf}(x)^3-18\big(4-2\pi+\sqrt{3}\,\pi\,\mathrm{erf}(\sqrt{3}x)\big)\Big] \\
& +\frac{1}{24\pi^3}\Big[120+\pi\Big\{90\sqrt{3}-104+\pi(12\pi+17\sqrt{3}+6)\Big\}+6\sqrt{3}\pi^2\,\mathrm{erf}(\sqrt{3}x)\Big]\mathrm{erfc}(x) \\
& -\frac{1}{8\pi^2}\{20+6(\sqrt{3}+2)\pi+13\pi^2\}\,\mathrm{erfc}(x)^2+\frac{1}{4\pi}(7\pi+6)\,\mathrm{erfc}(x)^3-\frac{15}{24}\,\mathrm{erfc}(x)^4 \\
& +\frac{\sqrt{3}}{8\pi^2}\Big\{(11\pi-18)\,\mathrm{erfc}(\sqrt{3}x)-128\pi\,T\left(\sqrt{6}x,\frac{1}{\sqrt{3}}\right)\Big\}. \qquad (2.56)
\end{aligned}
$$

This explicit expression for $\phi_3(x)$ seems to be new, not available in literature.

3 Discussion

The main goal of this report is the derivation of the explicit expressions for the second and third order corrections in the approximation of the modified error function which satisfies Eq.(1.1). Results presented here have been derived through the evaluation of integrals involving error-, exponential- and algebraic functions. The plots of successive corrections $\phi_i(x),\ 0 \leq i \leq 3$ show that the order of magnitude is decreasing term by term with $\mid \frac{\phi_{n+1}}{\phi_n} \mid \leq \frac{1}{2}$. It indicates that the series in (1.3) seems to converge for $\delta \leq 2$. Most of the results obtained here appear to be new and resolve the uneasiness appearing in [1]. The results derived here may be useful for the researchers working in the field of Stefan problems. The limitation of this approximation scheme is that the derivation of the explicit expression for the next order corrections ($\phi_i(x),\ i \geq 4$) involves intricate calculations due to the presence of integrals containing Owen *T*-functions which are not even manageable with the help of symbolic computations in a straightforward way. Hence alternative approximation scheme for the modified error function $\Phi_\delta(x)$ with higher order accuracy is desirable.

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