

On The Generalized Mass Transfer with a Chemical Reaction: Fractional Derivative Model

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ABSTRACT: In this article using the inverse Laplace transform, we show analytical solutions for the generalized mass transfers with (and without) a chemical reaction. These transfers have been expressed as the Couette flow with the fractional derivative of the Caputo sense. Also, using the Hankel contour for the Bromwich's integral, the solutions are given in terms of the generalized Airy functions.

Keywords: Lévêque Problem, Laplace transform, Generalized Airy functions, Fractional derivative.

1. INTRODUCTION

The mass transfer operations play a critical role in chemistry and other related science especially in chemical engineering. These operations are closely connected with the analogous problems of the convective heat transfer from non-isothermal surfaces. When a system contains more than one component whose concentration varies from one location to another, there is a natural propensity for mass to be transferred. There are many transfer operations in the literature such as solid dissolving in a liquid, gas absorption in a liquid and etc. which provides wide class of researches in chemical and energy sciences. For example in [7], analytical solutions and asymptotic expressions are proposed for homogenous and heterogeneous chemical reactions. Elperin et al. [11] have been solved the problem of mass transfer with a heterogeneous chemical reaction of the first order in boundary layer flows on non-newtonian power-law fluids.

Luchko and Punzi presented physical behavior behind the anomalous processes described by the continuous time random walk (CTRW) model and discussed on its feasibility for modeling of heat transform processes heterogeneous media [13]. Also, they

deduce a macroscopic model in form of a generalized fractional diffusion equation from the CTRW model on the microscopic level. Oldham demonstrated that that the electric current is linearly related to the temporal semiderivative of the concentrations at the electrode of the species involved in the electrochemical reaction [14].

The problem of mass transfer with (without) an irreversible chemical reaction in different flows has been discussed in the literature and has been mostly presented in the Newtonian and non-Newtonian liquids, or in the case of permeable surfaces. This problem can be formulated in the following form [7], [9, 10], [11]

$$(b + \alpha y) \frac{\partial u}{\partial x} = D \frac{\partial^2 u}{\partial y^2} - ku, \quad D > 0, a, b, k \in \mathbf{R}, \quad (1-1)$$

$$u(0, y) = 0, u(x, 0) = u_0, \quad (1-2)$$

$$\lim_{y \rightarrow \infty} u(x, y) < \infty. \quad (1-3)$$

A short treatise of the above equation with different situations may be considered as [7]:

- In case $a = 0$ and $b \neq 0$, it is known as the uniform (plug) flow.
- In case $a \neq 0$ and $b = 0$, it is known as the Couette flow.
- In case $a \neq 0$ and $b \neq 0$, it is known as the Couette flow with moving interface.

For the above three cases, if we set $k = 0$, then this mass transfer is interpreted without a chemical reaction and for $k \neq 0$, it is considered as a homogenous chemical reaction. For solving this problem, the Laplace integral transform method has been proposed which leads to the analytical solutions with the closed form and corresponding asymptotic expressions. For these solutions, the Airy function of the first kind [19]

$$Ai(y) = \frac{1}{\pi} \int_0^\infty \cos(yr + \frac{r^3}{3}) dr, \quad (1-4)$$

plays an important role for determining the structures and forms of them. This function is appeared in the inverse Laplace transform of the Bromwich's integral on the Hankel contour, see Figure 1 and references [7],[18].

As generalization of the problem (1-1), in this paper, first we consider the following partial differential equation with the higher order derivatives

$$(b + \alpha y) \frac{\partial u}{\partial x} = D_n \frac{\partial^{2n} u}{\partial y^{2n}} - ku, \quad D_n = (-1)^{n+1}, a, b, k \in \mathbf{R}, n \in \bullet, \quad (1-5)$$

$$u(0, y) = 0, u(x, 0) = u_0, \quad (1-6)$$

$$\lim_{y \rightarrow \infty} u(x, y) < \infty. \quad (1-7)$$

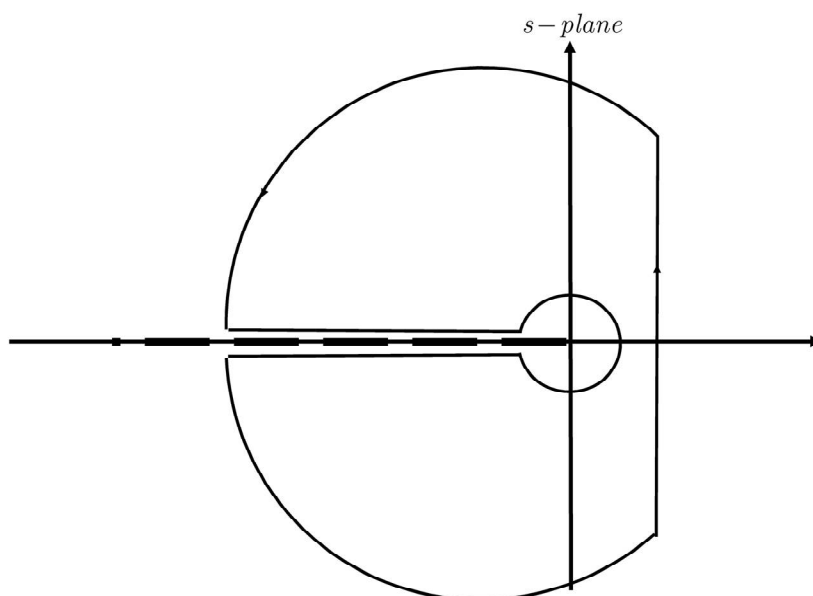


Figure 1. The Hankel Contour.

and show that the solution of this problem is written in terms of the generalized Airy function [1]

$$A_{2n+1}(y) = \frac{1}{\pi} \int_0^{\infty} \cos\left(yr + \frac{r^{2n+1}}{2n+1}\right) dr. \quad (1-8)$$

In second step, we modify the solution of problem (1-5) with respect to the fractional derivative in the Caputo sense [17]

$$({}^C D_x^\alpha f)(x) = \frac{1}{\Gamma(n-\alpha)} \int_0^x (x-s)^{n-\alpha-1} f^{(n)}(s) ds, \quad n-1 < \alpha \leq n, \quad (1-9)$$

for the following problem

$$(b + ay) {}^C D_a^\alpha u = D \frac{\partial^{2n} u}{\partial y^{2n}} - ku, \quad 0 < \alpha \leq 1. \quad (1-10)$$

To express our motivation, in Section 2 we survey the preliminaries properties of the generalized Airy functions (1-8) and in next sections we solve the problems (1-5) and (1-10) in different cases of parameters a, b, k using the Laplace transform. The solutions are obtained with respect to the Bromwich's integral on the Hankel contour in terms of the generalized Airy functions.

Table 1. Positive zeros of $A_{2n+1}(x)$ function for $n = 1, 2, 3, 4$.

| | | |
|---------|----------|--|
| $n = 1$ | $A_3(x)$ | - |
| $n = 2$ | $A_5(x)$ | $\lambda_{21} = 2.754254$ |
| $n = 3$ | $A_7(x)$ | $\lambda_{31} = 2.65450, \lambda_{32} = 5.35923$ |
| $n = 4$ | $A_9(x)$ | $\lambda_{41} = 2.65927, \lambda_{42} = 5.33275, \lambda_{43} = 7.97432$ |

2. THE GENERALIZED AIRY FUNCTIONS

The generalized Airy function (1–8) is the solution of ordinary differential equation of order $2n$

$$(-1)^{n+1} y^{(2n)} - xy = 0, \quad x \in \mathbb{P}. \quad (2-1)$$

This solution can be obtained using the Laplace integral method

$$y(x) = \int_C e^{xz} v(z) dz, \quad (2-2)$$

as

$$y(x) = \int_C e^{xz - \frac{z^{2n+1}}{2n+1}} dz, \quad (2-3)$$

where contour C is chosen such that the function $v(z)$ must vanish at boundaries. After deformation and normalization of integral (2-3), we rewrite the y as the $A_{2n+1}(x)$ function as follows

$$A_{2n+1}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ixz + i\frac{z^{2n+1}}{2n+1}} dz, \quad (2-4)$$

$$= \frac{1}{\pi} \int_0^{\infty} \cos(xz + \frac{z^{2n+1}}{2n+1}) dz, \quad (2-5)$$

with value [1]

$$A_{2n+1}(0) = \frac{\Gamma(\frac{1}{2n+1}) \cos(\frac{\pi}{2(2n+1)})}{(2n+1)^{\frac{2n}{2n+1}}}. \quad (2-6)$$

Figure 2 shows the behavior of the $A_{2n+1}(x)$ function for $n = 1, 2, 3, 4$ which is similar to the Airy function. It is obvious that the $A_{2n+1}(x)$ function has infinite negative roots on the negative semiaxes and $n-1$ positive roots on positive semiaxes, see Table 1

for some positive roots of the $A_{2n+1}(x)$ function. Also, for more applications and contributions of this function in partial fractional differential equations especially higher order heat equation

$$\frac{\partial}{\partial t} u(x,t) = \frac{\partial^n}{\partial x^n} u(x,t), \quad u(x,0) = u_0(x), \quad (2-7)$$

see [2-5], [6], [12] [15, 16].

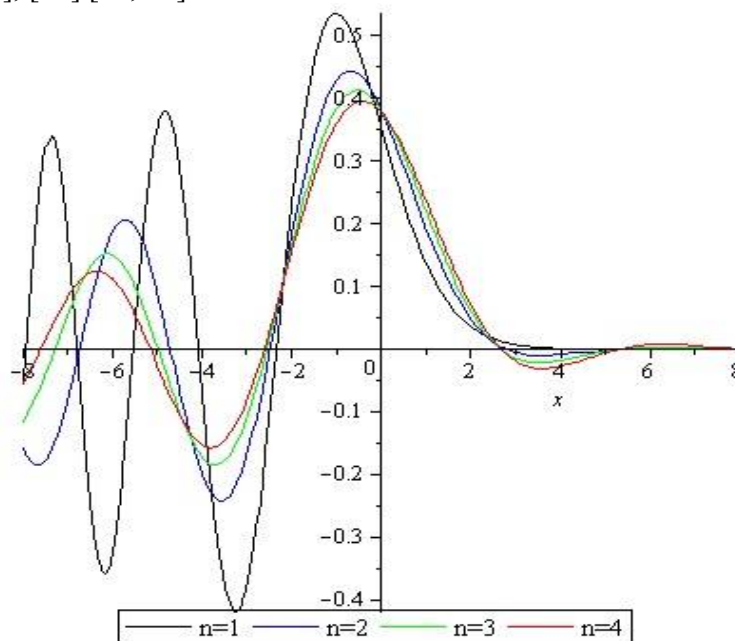


Figure 2. The generalized Airy functions for $n = 1,2,3,4$

3. THE GENERALIZED MASS TRANSFER IN COUETTE FLOW

In this section we start with a theorem for the inverse Laplace transform of multi-valued function $F(s)$. We assume that the point $s = 0$ is a branch point and F has no poles, then the inverse Laplace transform of $F(s)$, can be computed by means of the integral of a real-valued function.

Theorem 3.1 (Titchmarsh theorem [8]) Let $F(s)$ be an analytic function which has a branch cut on the real negative semiaxis, furthermore $F(s)$ has the following properties

$$F(s) = O(1), \quad |s| \rightarrow \infty,$$

$$F(s) = O\left(\frac{1}{|s|}\right), \quad |s| \rightarrow 0,$$

for any sector $|\arg(s)| < \pi - \eta$ where $0 < \eta < \pi$. Then the inverse Laplace transform of $F(s)$, can be written as the Laplace transform of the imaginary part of the function $F(re^{-i\pi})$

$$f(x) = L^{-1}\{F(s); x\} = \frac{1}{2\pi} \lim_{s \rightarrow 0} \int_{-\pi}^{\pi} \varepsilon F(\varepsilon e^{i\theta}) e^{i\theta + x\varepsilon e^{i\theta}} d\theta - \frac{1}{\pi} \int_0^{\infty} e^{-rx} \Im(F(re^{-i\pi})) dr. \quad (3-1)$$

3.1 THE COUETTE FLOW WITHOUT CHEMICAL REACTION: THE GENERALIZED LÉVÊQUE PROBLEM

Problem 3.2 *We consider a mass transfer without chemical reaction which is known as the Lévêque problem in the literature [7]. In this case we generalize and reformulate it with equation (1-5) as*

$$\frac{\partial u}{\partial x} = D_n \frac{\partial^{2n} u}{\partial y^{2n}}, \quad n \in \mathbb{N}, \quad (3-2)$$

$$u(0, y) = 0, u(x, 0) = u_0, \quad (3-3)$$

$$\lim_{y \rightarrow \infty} u(x, y) < \infty. \quad (3-4)$$

For solving this problem, we apply the Laplace transform on both sides of equation (3-2) with respect to x

$$\tilde{u}(s, y) = \int_0^{\infty} e^{-sx} u(x, y) dx, \quad (3-5)$$

and use the boundary condition to derive the relation

$$D_n \frac{\partial^{2n} \tilde{u}}{\partial y^{2n}} - s y \tilde{u} = 0. \quad (3-6)$$

In view of the finiteness of solution and $2n$ linear independent solutions of the above differential equation, we get the solution with respect to the $A_{2n+1}(x)$ function in the following form

$$\tilde{u}(s, y) = C(s) A_{2n+1}(s^{\frac{1}{2n+1}} y). \quad (3-7)$$

Applying other boundary condition, we obtain the unknown coefficient $C(s)$, that is

$$\tilde{u}(s, y) = \frac{u_0}{s A_{2n+1}(0)} A_{2n+1}(s^{\frac{1}{2n+1}} y). \quad (3-8)$$

The inverse of (3-8) is obtained by considering the Bromwich's integral

$$u(x, y) = \frac{u_0}{2\pi i A_{2n+1}(0)} \int_{c-i\infty}^{c+i\infty} \frac{1}{s} A_{2n+1}(s^{\frac{1}{2n+1}} y) e^{sx} ds, \quad (3-9)$$

which has a branch point at the origin. By using the suitable change of the Bromwich contour of integration (Figure 1) and applying the Titchmarsh Theorem 3.1, we get the solution as

$$u(x, y) = u_0 - \frac{u_0}{\pi A_{2n+1}(0)} \int_0^\infty \frac{1}{r} e^{-rx} \Im \{ A_{2n+1}(r^{\frac{1}{2n+1}} e^{-i\frac{\pi}{2n+1}y}) \} dr. \quad (3-10)$$

For simplification of the above solution for $n = 1$ in terms of the Bessel functions, first consider the following identity in terms of the modified Bessel functions [7]

$$Ai(x) = \frac{\sqrt{x}}{3} (I_{-\frac{1}{3}}(\frac{2}{3}x^{\frac{3}{2}}) - I_{\frac{1}{3}}(\frac{2}{3}x^{\frac{3}{2}})),$$

and use the Theorem 3.1 to obtain the solution in terms of the imaginary parts of Airy function as follows

$$u(x, y) = u_0 - \frac{u_0 3^{\frac{1}{6}} \Gamma(\frac{2}{3})}{2\pi} \int_0^\infty \frac{1}{r^{\frac{5}{6}}} e^{-rx} y^{\frac{1}{2}} J_{\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}}y^{\frac{3}{2}}) dr. \quad (3-11)$$

Also, the solution of equation (3-2), can be generalized by replacing the term $\frac{\partial u}{\partial x}$ by ${}^C D_x^\alpha u$ as the Caputo fractional derivative. In the sense, by using the fact [17]

$$\Lambda \{ {}^C D_x^\alpha u(x, y); s \} = s^\alpha \tilde{u}(s, y) - s^{\alpha-1} u(0, y), \quad 0 < \alpha \leq 1, \quad (3-12)$$

and applying the similar procedure for solving the new problem, we obtain the solution (3-10) in the following form

$$u(x, y) = u_0 - \frac{u_0}{\pi A_{2n+1}(0)} \int_0^\infty \frac{1}{r} e^{-rx} \Im \{ A_{2n+1}(r^{\frac{\alpha}{2n+1}} e^{-i\frac{\pi}{2n+1}y}) \} dr. \quad (3-13)$$

Problem 3.3 We consider other type of the generalized Lévêque problem as

$$(1 + y) \frac{\partial u}{\partial x} = D_n \frac{\partial^{2n} u}{\partial y^{2n}}, \quad n \in \mathbb{N}, \quad (3-14)$$

$$u(0, y) = 0, u(x, 0) = u_0, \quad (3-15)$$

$$\lim_{y \rightarrow \infty} u(x, y) < \infty. \quad (3-16)$$

In similar procedure to the previous problem, after applying the Laplace transform we get

$$\tilde{u}(s, y) = \frac{u_0}{s A_{2n+1}(s^{\frac{1}{2n+1}}(1 + y))}, \quad (3-17)$$

which its inverse is obtained by the following Bromwich's integral

$$u(x, y) = \frac{u_0}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{1}{s A_{2n+1}(s^{\frac{1}{2n+1}}y)} e^{sx} ds. \quad (3-18)$$

The integrand of the Bromwich's integral has the branch point at the origin and infinite number of poles s_n as

$$A_{2n+1}(s_j^{\frac{1}{2n+1}}) = A_{2n+1}(\lambda_{nj}) = 0, j = 1, 2, \dots, \tag{3-19}$$

where λ_{nj} are the zeros of the A_{2n+1} function. It is evident that the all poles $s_j = \lambda_{nj}^{2n+1}$ are outside the contour of integration except $n-1$ positive roots of them. Some of these positive zeros has been shown in Table 1. Therefore, for obtaining the residues at the simple poles $s_j, j = 1, \dots, n-1$, we have

$$\begin{aligned} I_n &= \sum_{i=1}^{n-1} Res\left\{ \frac{1}{sA_{2n+1}(s^{\frac{1}{2n+1}})} A_{2n+1}(s^{\frac{1}{2n+1}}y)e^{sx}; s_i = \lambda_{ni}^{2n+1} \right\} \\ &= \sum_{i=1}^{n-1} \frac{(2n+1)}{\lambda_{ni}A_{2n+1}'(\lambda_{ni})} A_{2n+1}(\lambda_{ni}y)e^{\lambda_{ni}^{2n+1}x}. \end{aligned} \tag{3-20}$$

According to the above value and Titchmarsh theorem, we finally get the solution of Problem 2 as

$$u(x, y) = (1 + I_n)u_0 - \frac{u_0}{\pi} \int_0^\infty \frac{1}{r} e^{-rx} \Im \left\{ \frac{A_{2n+1}(r^{\frac{1}{2n+1}}e^{-i\frac{\pi}{2n+1}}y)}{A_{2n+1}(r^{\frac{1}{2n+1}}e^{-i\frac{\pi}{2n+1}})} \right\} dr. \tag{3-21}$$

Also, in the case of the fractional derivative model of problem with respect to x , we get the solution of problem in the following form

$$u(x, y) = (1 + I_{n,\alpha})u_0 - \frac{u_0}{\pi} \int_0^\infty \frac{1}{r} e^{-rx} \Im \left\{ \frac{A_{2n+1}(r^{\frac{1}{2n+1}}e^{-i\frac{\pi}{2n+1}}y)}{A_{2n+1}(r^{\frac{1}{2n+1}}e^{-i\frac{\pi}{2n+1}})} \right\} dr, \tag{3-22}$$

where

$$I_{n,\alpha} = \sum_{i=1}^{n-1} \frac{(2n+1)}{\alpha\lambda_{ni}A_{2n+1}'(\lambda_{ni})} A_{2n+1}(\lambda_{ni}y)e^{\lambda_{ni}^{\frac{2n+1}{\alpha}}x}. \tag{3-23}$$

For simplification of the solution (3-21) in $n = 1$ in terms of the Bessel functions, similar to the previous procedure in (3-11), we use Theorem 3.1 to obtain

$$u(x, y) = u_0 - \frac{u_0 3^{\frac{1}{2}}(1+y)^{\frac{1}{2}}}{2\pi} \int_0^\infty \frac{1}{r} e^{-rx} \frac{J_{\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}}(1+y)^{\frac{3}{2}})J_{\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}}) - J_{\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}}(1+y)^{\frac{3}{2}})J_{\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}})}{J_{\frac{1}{3}}^2(\frac{2}{3}r^{\frac{1}{2}}) + J_{\frac{1}{3}}^2(\frac{2}{3}r^{\frac{1}{2}}) - J_{\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}})J_{\frac{1}{3}}(\frac{2}{3}r^{\frac{1}{2}})} dr \tag{3-24}$$

3.2. THE COUETTE FLOW WITH A CHEMICAL REACTION

At this point, we consider the Couette flow in the presence of a chemical reaction.

Problem 3.4 We consider the following Couette flow with a chemical reaction

$$y \frac{\partial u}{\partial x} = D_n \frac{\partial^{2n} u}{\partial y^{2n}} - u, n \in \mathbb{N}, \tag{3-25}$$

$$u(0, y) = 0, u(x, 0) = u_0, \tag{3-26}$$

$$\lim_{y \rightarrow \infty} u(x, y) < \infty. \tag{3-27}$$

For this problem similar to the previous problem, after applying the Laplace transform and boundary conditions, we get the solution as

$$\tilde{u}(s, y) = \frac{u_0}{sA_{2n+1} \left(\frac{1}{\frac{2n}{s^{2n+1}}} \right)} A_{2n+1} \left(\frac{1+sy}{\frac{2n}{s^{2n+1}}} \right). \tag{3-28}$$

In view of the $n-1$ positive simple poles $s_i = \frac{1}{\lambda_{ni}^{2n}}, i = 1, 2, \dots, n-1$, the inverse Laplace transform of the above function is given by

$$u(x, y) = (1 + I_n)u_0 - \frac{u_0}{\pi} \int_0^\infty \frac{1}{r} e^{-rx} \Im \left\{ \frac{A_{2n+1} \left[\frac{1 + re^{-i\pi}}{\frac{2n}{r^{2n+1}}} \right]}{A_{2n+1} \left[\frac{1}{\frac{2n}{(re^{-i\pi})^{2n+1}}} \right]} \right\} dr, \tag{3-29}$$

where

$$I_n = \sum_{i=1}^{n-1} \text{Res} \left\{ \frac{A_{2n+1} \left(\frac{1+sy}{\frac{2n}{s^{2n+1}}} \right)}{sA_{2n+1} \left(\frac{1}{\frac{2n}{s^{2n+1}}} \right)} e^{sx}; s_i = \frac{1}{\lambda_{ni}^{2n}} \right\}$$

$$= - \sum_{i=1}^{n-1} \frac{(2n+1)}{2n\lambda_{ni} A_{2n+1}'(\lambda_{ni})} A_{2n+1} \left(\frac{1 + \frac{y}{\frac{2n}{\lambda_{ni}^{2n}}}}{\frac{2n}{\lambda_{ni}^{2n}}} \right) e^{\lambda_{ni}^{2n} x}. \tag{3-30}$$

Also, in the case of the fractional derivative model of problem, we get the solution of problem in the following form

$$u(x, y) = (1 + I_n)u_0 - \frac{u_0}{\pi} \int_0^\infty \frac{1}{r} e^{-rx} \Im \left\{ \frac{A_{2n+1} \left[\frac{1 + r^\alpha e^{-i\pi\alpha} y}{(re^{-i\pi})^{2n+1}} \right]}{A_{2n+1} \left[\frac{1}{(re^{-i\pi})^{2n+1}} \right]} \right\} dr, \quad (3-31)$$

where

$$I_{n,\alpha} = - \sum_{i=1}^{n-1} \frac{(2n+1)}{2n\alpha\lambda_{ni} A_{2n+1}'(\lambda_{ni})} A_{2n+1} \left(\frac{1 + \frac{y}{\lambda_{ni}^{2n\alpha}}}{\lambda_{ni}} \right) e^{\left(\frac{x}{\lambda_{ni}^{2n\alpha}} \right)}. \quad (3-32)$$

Moreover, for simplification of the solution (3-29) in $n=1$ in terms of the Bessel functions, we get

$$u(x, y) = u_0 e^{-y} - \frac{u_0 3^{\frac{1}{2}}}{2\pi} \int_0^\infty \frac{(1-ry)^{\frac{1}{2}}}{r} e^{-rx} \frac{J_1\left(\frac{2}{3r}(1-ry)^{\frac{3}{2}}\right) J_{-\frac{1}{3}}\left(\frac{2}{3r}\right) - J_{-\frac{1}{3}}\left(\frac{2}{3}(1-ry)^{\frac{3}{2}}\right) J_1\left(\frac{2}{3r}\right)}{J_1^2\left(\frac{2}{3r}\right) + J_{-\frac{1}{3}}^2\left(\frac{2}{3r}\right) - J_{-\frac{1}{3}}\left(\frac{2}{3r}\right) J_1\left(\frac{2}{3r}\right)} dr. \quad (3-33)$$

4. CONCLUDING REMARKS

This paper provides new results in obtaining the analytical solutions of some generalized partial differential equations. These equations have been interpreted as the Couette flows with (without) chemical reactions. We considered fractional derivative models (in Caputo sense) for these PDEs and solved them by the Laplace transform. We encountered with the generalized Airy functions in the Bromwich's integral of inverse Laplace transform. Zeros of these functions were the first steps in obtaining the solutions as the simple poles of integrands. Finally, the desired solutions have been written in terms of the Laplace transform of the imaginary parts of the generalized Airy functions.

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