

STARTING RADIAL SUBDIFFUSION FROM A CENTRAL POINT THROUGH A DIVERGING MEDIUM (A SPHERE): Heat-Balance Integral Method

by

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The work presents an integral solution of the time-fractional subdiffusion equation as alternative approach to those employing hypergeometric functions. The integral solution suggests a preliminary defined profile with unknown coefficients and the concept of penetration (boundary layer) well known from the heat diffusion and hydrodynamics. The profile satisfies the boundary conditions imposed at the boundary of the boundary layer that allows its coefficients to be expressed through the boundary layer depth as unique parameter describing the profile. The technique is demonstrated by a solution of a time fractional radial equation concerning anomalous diffusion from a central point source in a sphere.

Key words: radial subdiffusion, integral method, heat-balance integral, fractional Fourier number

Introduction

The subdiffusion process has been observed in many real physical systems such as highly ramified media in porous systems [1-4], anomalous diffusion in fractals [5], diffusion in thick membranes [6], anomalous drug absorption and disposition processes [7], heat transfer close to equilibrium [8], etc. Subdiffusion occurs in a variety of applications as discussed in the review papers [9-11]. For the problem presented here, it is convenient to think of the application to certain porous materials in which microscopic pores are filled with a substance that has a lower conductivity than that of the basic matrix material as described in [2, 12]. The underlying physics of subdiffusion is associated with a medium in which the mean square displacement of Brownian motion evolves on a slower-than-normal time scale, that is $\langle X^2 \rangle \sim t^\mu$, where the anomalous diffusion parameter μ is within the range $0 < \mu < 1$. A continuum model of a subdiffusive material is consistent with the scenario in which the pore size is small in comparison to $\langle X^2 \rangle^{1/2}$ [1].

There has been a growing interest to investigate the solutions of subdiffusive equations and their properties for various reasons which include modeling of anomalous

diffusive and subdiffusive systems, description of fractional random walk, unification of diffusion and wave propagation phenomenon, and simplification of the results. The common methods for solving fractional-order equations are purely mathematical [13], even though they are approximate in nature, among them: in terms of Mittag-Leffler function [14], similarity solutions [15], Green's function [16, 17], operational calculus [18], numerical methods [19], variational iteration method [20, 21], and differential transformations [22, 23].

The present work refers to an integral solution commonly known as heat-balance integral [24, 25]. The core of the model is the assumption of the thermal penetration layer propagating with a finite velocity. Beyond the front of this layer the medium is undisturbed. This idea of Goodman [24], in fact, corrects the physical incorrectness of the parabolic heat-equation where the speed of the flux is infinite. The integral solution suggests a prescribed profile with unknown coefficients satisfying the boundary conditions at the both ends of the penetration layer. The integral approach to the fractional equation suggests replacement of the real function by an approximate profile and integration over the penetration depth. The technique was demonstrated recently [26] in a solution of a half-time fractional equation resulting by splitting of the normal (diffusion) parabolic equation and Riemann-Liouville time-derivative.

The specific case of time-fractional radial subdiffusion is an example demonstrating the technique of the integral method, because it is possible to transform the radial diffusion equation into 1-D time-fractional subdiffusion equation [27], to which the method was already applied [26].

There are few solutions of the radial subdiffusion in a sphere [28], cylinder [14, 29], hollow geometries (including a spherical shell) [27], expressed through Caputo derivatives and the Mittag-Leffler function even though the methods are different, among them: Separation of variables and Laplace transform [27], Hankel transform [14], Grünwald-Letnikov numerical algorithm [29], sin-Fourier transform [28]. All these existing solutions form a background allowing demonstrating the features of the integral method.

The integral method – mathematical formulation

It is assumed that the temperature (concentration) $T(x, t)$ in the semi-infinite subdiffusive material satisfies the one-dimensional fractional diffusion equation given by:

$$\frac{\partial^\mu T(x, t)}{\partial t^\mu} = a \frac{\partial^2 T(x, t)}{\partial x^2} \quad (1a)$$

$$T(0, t) = T_s, \quad t \geq 0; \quad T(x, 0) = T_\infty, \quad x > 0; \quad \frac{\partial T(x, 0)}{\partial t} = 0, \quad x > 0, \quad (1b, c, d)$$

$$\frac{d^\mu T}{dt^\mu} = {}_{RL}D_t^\mu T(x, t) = \frac{1}{\Gamma(1-\mu)} \frac{d}{dt} \int_0^t \frac{T(x, u)}{(t-u)^\mu} du \quad (1e)$$

where a_μ is a sort of fractional diffusion coefficient of dimensions $a_\mu = [m^2/s^\mu]$ and (1e) is the Riemann-Liouville fractional derivative of $T(x, t)$ with respect to the time t [18].

Commonly (1a) is solved by shifting to the Caputo representation of fractional derivatives because when the Laplace transform method is applied the resulting problem gets a boundary condition containing the limit value of the Riemann-Liouville fractional

derivatives at $t = 0$ that has not a physical background. The Laplace transform of the Caputo derivative imposes boundary conditions involving integer-order derivatives at the lower point $t = 0$ which usually are acceptable physical conditions. Another advantage is that the Caputo derivative of a constant is zero, whereas for the Riemann-Liouville is not. However, the following analysis suggest an alternate integral approach where the main reason to use the Caputo derivative is avoided and the solution of the sub-diffusion equation is developed in the form of Riemann-Liouville presentation.

As it was mentioned at the beginning, the integral approach considers a finite depth of penetration δ of the temperature (concentration) into the medium, which evolve in time, *i. e.* $\delta(t)$. Beyond the point $x = \delta(t)$, the medium is undisturbed and:

$$T(x, \delta) = T_{\infty}, x > \delta \quad (2a)$$

$$\frac{\partial T(\delta, t)}{\partial x} = 0, \delta(t) = 0, \quad t = 0 \quad (2b,c)$$

This approach is supported by experimental facts of almost sharp fronts of penetration of the diffusion substances [6, 7, 30, 31]. Moreover, the fractional diffusion equation referring sub-diffusion problems [6] the heat (mass) propagation (diffusion) is so slow [8, 31, 32] that the concept of the penetration layer becomes essential in view of the fact that it really exists [6, 7, 30, 31]. In accordance with the heat-balance concept at any time t the integral of both sides (1a) along δ should be:

$$\int_0^{\delta} \left[\frac{\partial^{\mu}}{\partial t^{\mu}} T(x, t) \right] dx = a_{\mu} \int_0^{\delta} \frac{\partial^2 T(x, t)}{\partial x^2} dx \quad (3a)$$

That yields

$$\int_0^{\delta} \left[\frac{\partial^{\mu}}{\partial t^{\mu}} T(x, t) \right] dx = a_{\mu} \left. \frac{\partial T}{\partial x} \right|_{x=0}^{\delta} \quad (3b)$$

The integral of left-side in (3a, b) is termed hereafter – **fractional-time heat-balance integral (FT-HBI)** following [26]. If the distribution $T(x, t)$ across the penetration is approximated by $T_a(x)$ depending only on x , $0 < x < \delta(t)$ and the boundary conditions (2a, b) and (1b) are applied, then we get a profile (distribution) expressed as a function of x and coefficients depending on $\delta(t)$. Further, replacing $T(x, t)$ by the $T_a(x, \delta)$, in (3b) we get:

$$\int_0^{\delta} \left[\frac{\partial^{\mu}}{\partial t^{\mu}} T_a(x, \delta(t)) \right] dx = a_{\mu} \left. \frac{\partial T_a(x, \delta(t))}{\partial x} \right|_{x=0}^{\delta} \quad (4)$$

Now, the main problem is the evaluation of the fractional heat-balance integral (4) through particular expression of $T_a(x, \delta)$ and the definition of the fractional-time derivative:

$${}_{RL}D_t^{\mu} T_a(x, \delta(t)) = \frac{1}{\Gamma(1-\mu)} \frac{d}{dt} \int_0^t \frac{T_a(x, \delta(\tau))}{(t-\tau)^{\mu}} d\tau \quad (5)$$

The crux of the heat-balance integral is the left-hand side of (3a) and (4) since the distribution $T(x, t)$ should satisfy the integral in average, but not the original domain equation (1a). The second principle point is the choice of the approximating profile $T_a(x)$, which is

commonly expressed as a polynomial function of integer order: quadratic or cubic [24, 25]. Here we will use a generalized parabolic profile $T_a(x, t) = b_1 + b_2(1 + b_3x)^n$ with unspecified exponent [26-28] and $T(0, t) = T_s$ as boundary condition at $x = 0$. Applying the boundary conditions (2a, b) and (1b) to the approximate profile we get:

$$T_a(x, t) = T_\infty + (T_s - T_\infty) \left(1 - \frac{x}{\delta}\right)^n \Rightarrow \Theta_a(x, t) = \frac{T - T_\infty}{T_s - T_\infty} = \left(1 - \frac{x}{\delta}\right)^n \quad (6)$$

The exponent n is still unspecified and its exact value (non-integer) will be discussed further in this work. Now, we turn to the time-fractional radial sub-diffusion equation.

Time-fractional radial subdiffusion

Consider time-fractional radial subdiffusion in a spherical shell $R_1 < r < R_2$

$$\frac{\partial^\mu T}{\partial t^\mu} = a_\mu \left(\frac{\partial^2 T}{\partial r^2} + 2 \frac{\partial T}{\partial r} \right), \quad t > 0 \quad (7)$$

The initial and boundary conditions to (7) are:

$$T = T_\infty, \quad t = 0, \quad 0 < \mu < 1; \quad \frac{\partial T}{\partial t} = 0, \quad t = 0, \quad 0 < \mu < 1 \quad (8a, b)$$

$$T(R_1, t) = T_s, \quad T(R_2, t) = T_\infty, \quad \frac{\partial T(\delta, t)}{\partial r} = 0, \quad \delta(t) < \Delta R = R_2 - R_1 \quad (8c, d, e)$$

The problem of normal diffusion ($\mu = 1$) with the substitution $U(r, t) = rT(r, t)$ [26] is:

$$\frac{\partial U}{\partial t} = a_\mu \frac{\partial^2 U}{\partial r^2} \quad (9a)$$

With the profile $U(r, t) = \beta_0 + \beta_1(1 + \beta_2 r)^n$ satisfying the conditions:

$$U(R_1, t) = U_s, \quad U(\delta, t) = U_\infty, \quad \left. \frac{\partial U}{\partial r} \right|_{r=\delta} = 0 \quad (9b, cd)$$

yields [26]:

$$U(r, t) = U_\infty + (U_s - U_\infty) \left(\frac{\delta - r}{\delta - R_1} \right)^n, \quad \text{and with } U(r, t) \rightarrow T(r, t), \quad \Theta_a(r, t) = \left(\frac{\delta - r}{\delta - R_1} \right)^n \quad (9e, f)$$

The heat-balance integral solution in [26] defines $\delta(t)$ as a solution of:

$$\frac{d(\delta - R_1)^2}{dt} = 2an(n+1) \quad \text{with} \quad \delta - R_1 = 0 \quad \text{at} \quad t = 0 \quad (10a)$$

$$\text{That yields} \quad (\delta - R_1) = \sqrt{\alpha t} \sqrt{2n(n+1)} \quad (10b)$$

The final approximate profile is (9f) with $n = 2/(\pi - 2) \approx 1.75$ obtained through calibration at the exact solution of (9a) at $r = 0$.

Qui and Liu [27] solved (7) at $0 < \mu \leq 2$, through the following dimensionless variables:

$$u = \left(\frac{T - T_\delta}{T_{R_1} - T_{R_2}} \right) \frac{r}{R_2} = \left(\frac{T - T_\infty}{T_S - T_\infty} \right) \frac{r}{R_2}, \quad z = \frac{r - R_1}{R_2 - R_1}, \quad \tau_1 = t \left(\frac{a}{l_R^2} \right)^{1/\mu}, \quad l_R = R_2 - R_1 \quad (11)$$

transformed the problem to (solved by separation of variables):

$$\frac{\partial^\mu u}{\partial \tau_1^\mu} = \frac{\partial^2 u}{\partial y^2}, \quad 0 < z < 1, \quad \tau_1 > 0, \quad (12a)$$

$$\tau_1 = 0, \quad u = 0, \quad 0 < \mu \leq 2; \quad \tau_1 = 0, \quad \frac{\partial u}{\partial \tau_1} = 0, \quad 0 < \mu \leq 2 \quad (12b,c)$$

$$\left(\frac{\partial u}{\partial z} - hu \right) \Big|_{z=0} = 0, \quad u(1, \tau_1) = 1 \quad h = \lambda - 1 = \frac{R_2 - R_1}{R_1} \quad (12d)$$

We will avoid the complete adimensionalization of eq. (7) since the heat-balance integral solution allows the profile to be expressed through its own *length scale*. This implies, that with $\mu = 1$, for example, the length scale is $l_{\mu=1} \sim (at)^{1/2}$ and $\Theta_a(x, t) = (1 - x/\delta)^n$, with $\delta = (at)^{1/2} F(n)$. $F(n)$ is a function on of the exponent and depends on the boundary conditions applied at $x = 0$ [26, 33]. At the begging, the penetrating layer $\delta(t) < \Delta R = R_2 - R_1$ and the problem can be considered as a subdiffusion in a semi-infinite medium. Then, the transformation $C(r, t) = rT(r, t)$ the right-hand side of (7) can be transformed, that yields:

$$\frac{\partial^\mu C}{\partial t^\mu} = a_\mu \frac{\partial^2 C}{\partial r^2} \quad (13)$$

$$C(R_1, t) = C_s, \quad C(\delta, t) = C_\infty, \quad \frac{\partial C}{\partial r} \Big|_{r=\delta} = 0 \quad (13b,c,d)$$

With the transform $C(r, t) = rT(r, t)$, we get $(\partial C/r) \Big|_{r=\delta} = T(\delta, t) + \delta(T/r) \Big|_{r=\delta} = T_\infty$. Applying the parabolic profile $C(r, t) = \beta_0 + \beta_1(1 + \beta_2 r)^n$ and the conditions (9b) and assuming $C(r, t)$ instead $U(r, t)$ we have the approximate profile (see eq. 9d):

$$C_a^*(r, t) = \frac{C - C_\infty}{C_s - C_\infty} = \left(\frac{\delta - r}{\delta - R_1} \right)^n \quad (14)$$

Fractional-time heat-balance integral

The next important step is to evaluate the time-fractional derivative of (13) replacing $C(r, t)$ by the approximate distribution $C_a^*(r, t)$, that is, the following integral has to be solved:

$$I_{fr} = \int_0^\delta \left[\frac{\partial^\mu}{\partial t^\mu} C_a(x, t) \right] dx \quad (15)$$

The problems was developed in [26] and the solution of (15) with $\mu = 1/2$ is:

$$I_{fr}^a \left(\frac{1}{2} \right) = \frac{d}{dt} \left[\int_0^t du \int_0^\delta \frac{\left(1 - \frac{x}{\delta} \right)^n}{\sqrt{t-u}} dx \right] \Rightarrow \frac{d}{dt} \left[\int_0^t \left(\frac{\delta}{n+1} \right) \frac{1}{\sqrt{t-u}} du \right] \Rightarrow \frac{2}{\sqrt{\pi}} \frac{1}{n+1} \frac{d}{dt} (\delta \sqrt{t}) \quad (16)$$

Following the same technique (see details about the integration in ref. [26]) at any $0 < \mu < 1$ we get from the definition (1e) the following approximation of the time-fractional derivative $\partial^\mu C_a^* / \partial t^\mu$, namely:

$$I_{fr(\mu)}^a = \frac{d}{dt} \left[\int_0^t du \int_0^\delta \frac{\left(1 - \frac{r}{\delta}\right)^n}{(t-u)^\mu} dr \right] \Rightarrow \frac{d}{dt} \left[\int_0^t \left(\frac{\delta}{n+1}\right) \frac{1}{(t-u)^\mu} du \right] \Rightarrow \frac{1}{(1-\mu)} \frac{1}{n+1} \frac{d}{dt} (\delta t^{1-\mu}) \quad (17a)$$

That is, the approximation of $\partial^\mu C_a^* / \partial t^\mu$ by C_a^* yields:

$$\frac{\partial^\mu C_a^*(r,t)}{\partial t^\mu} = \frac{1}{\Gamma(1-\mu)} \left[\frac{1}{(1-\mu)} \frac{1}{n+1} \frac{d}{dt} (\delta t^{1-\mu}) \right] \quad (17b)$$

According to (3b) and the boundary conditions (13b, c, d), we have. Then, the heat-balance integral approximation of eq. (13) provides the following equation about $\delta(t)$ $\delta(t=0) = 0$.

$$\frac{d}{dt} (\delta t^{1-\mu}) - a_\mu \frac{N}{\delta} = 0, \quad (18a)$$

$$N = n(n+1)(1-\mu)\Gamma(1-\mu), \quad a_\mu \left(\frac{\partial C_a^*}{\partial r} \right)_{r=0} = \frac{n}{\delta} \quad (18b,c)$$

The new variable $\delta t^{1-\mu} = Z(t)$, transforms (18a) into:

$$Z \frac{d}{dt} Z - a_\mu N t^{1-\mu} = 0 \Rightarrow \frac{d}{dt} Z^2 = 2a_\mu N t^{1-\mu} \Rightarrow Z^2 = a_\mu \frac{2N}{2-\mu} t^{2-\mu} + C_1 \quad (19a)$$

$$\delta t^{1-\mu} = \sqrt{a_\mu} \sqrt{\frac{2N}{2-\mu}} t^{\frac{2-\mu}{2}} + \sqrt{C_1} \Rightarrow \delta = \sqrt{a_\mu} \sqrt{\frac{2N}{2-\mu}} \frac{t^{\frac{\mu}{2}}}{t^{1-\mu}} + \frac{\sqrt{C_1}}{t^{1-\mu}} \quad (19b)$$

The initial condition $\delta(t) = 0$ leads to $C_1 = 0$, which is a physically defined requirement relevant to the fact that the source providing the heat (mass) at $x = 0$ is of finite power and the heat(mass) penetrates slowly into the medium. From (19b), we have that $\delta_\mu \equiv (a_\mu t^\mu)^{1/2}$, thus defining the new length scale of the subdiffusion. From (19b) and the backward transform $C(r, t) \rightarrow rT(r, t)$, the approximate profile can be expressed as:

$$\Theta_a(r, t) = \frac{T - T_\infty}{T_s - T_\infty} = \left(\frac{\delta - r}{\delta - R_1} \right)^n = \left(\frac{1 - \frac{r}{\delta}}{1 - \frac{R_1}{\delta}} \right)^n \Rightarrow \left(1 - \frac{r}{\delta} \right)^n_{R_1=0} \quad (20a,b)$$

Fractional penetration depth

For simplicity of the next analysis, we will assume hereafter that $R_1 = 0$, that implies **a point source** of heat (mass) at $r = 0$. In this context, $R_2 = R$ (sphere radius) for seek of simplicity of the expressions. With T_s at $r = 0$, we have $\Theta(r, t) = (1 - r/\delta)^n$ (see 20,b). Further, from (19b) we get:

$$\Theta_a(r, t) = \left(1 - \frac{r}{\sqrt{a_\mu t^\mu} F_n j_\mu} \right)^n, \quad F_n = \sqrt{2n(n+1)}, \quad j_\mu = \sqrt{\frac{\Gamma(2-\mu)}{2-\mu}}, \quad (21)$$

The function F_n depends only on the exponent of the profile, while j_μ is a fractional correction factor. The product $F_n j_\mu$ shows how the penetration depth $\delta_\mu(t)$ of the subdiffusion varies with the fractional power μ , namely: (1) with a normal diffusion and $\mu = 1$ the heat-balance integral [33] provides $\delta(t) = (at)^{1/2} [2n(n+1)]^{1/2}$, i. e., $j_\mu = 1, 2$); (2) with $0 < \mu < 1$, $\delta_\mu(t) = (a_\mu t^\mu)^{1/2} F_n j_\mu$.

Calibration of the profile exponent

The final step in defining the approximate profile is the determination of the exponent n . It cannot be determined directly from the boundary conditions provided by the thermal layer concept. More exactly, the conditions (9c) and (9d) are valid at any n . The profile has four unknown parameters: three of them can be obtained from the existing boundary conditions at any n [4]. The problem requires an additional boundary condition at $x = 0$ defined through the so-called entropy minimization approach [34], namely. This additional boundary condition at $x = 0$ can be provided if an exact solution exists [34]. The solution developed next address a profile that satisfies the domain equation minimizing the mean-square error of approximation over the entire penetration layer.

Mean-square error approach

The approximate should satisfy the domain equation, so the mean-square error of approximation should be minimal. Hence, with the transformation $C(r, t) = rT(r, t)$ we have:

$$E_\mu(t) \equiv \int_0^{\delta(t)} \left[\frac{\partial^\mu}{\partial t^\mu} C_a(x, t) - a_\mu \frac{\partial^2 C_a}{\partial x^2} \right]^2 dx \geq 0, \quad E_\mu(t) \rightarrow \min \quad (22)$$

$$e_\mu(x, t) = \frac{\partial^\mu}{\partial t^\mu} C_a(x, t) - a_\mu \frac{\partial^2 C_a}{\partial x^2} \quad \text{and} \quad E_\mu(t) \equiv \int_0^{\delta(t)} [e_\mu(x, t)]^2 dx \quad (23a, b)$$

Further, with the dimensionless profile (20b) we have (see the expression (17b) for $\partial^\mu / \partial t^\mu$):

$$\frac{\partial^\mu}{\partial t^\mu} \Theta_a(x, t) = \left[\frac{1}{\Gamma(1-\mu)} \frac{1}{(1-\mu)} \frac{1}{n+1} \right] \left[t^{1-\mu} \frac{d\delta}{dt} + \delta(1-\mu)t^{-\mu} \right] \quad (24a)$$

$$\frac{\partial^2 \Theta_a}{\partial x^2} = \frac{n(n-1)}{\delta^2} \left(1 - \frac{x}{\delta} \right)^{n-2} \quad (24b)$$

$$e_\mu(x, t) = \left[\frac{1}{\Gamma(2-\mu)} \frac{1}{n+1} \right] \left[t^{1-\mu} \frac{d\delta}{dt} + \delta(1-\mu)t^{-\mu} \right] + \frac{n(n-1)}{\delta^2} \left(1 - \frac{x}{\delta} \right)^{n-2} \quad (24c)$$

The integration of (24) with $\delta_\mu = (a_\mu t^\mu)^{1/2} F_n j_\mu$, $d\delta_\mu/dt = (-\mu/2)t^{(-\mu/2)-1}(a_\mu)^{1/2} F_n j_\mu$, gives $E_\mu(t)$, namely:

$$E_\mu(t) = \frac{1}{\sqrt{at^\mu}} \left[G(n, \mu)(at^{\mu-1})F_n j_\mu + a \frac{\sqrt{at^\mu}}{t^\mu} (1-\mu)F_n^2 j_\mu^2 + 2a^2(1-\mu)F_n^3 j_\mu^3 - \right. \\ \left. -2G(n, \mu) \frac{at^{\mu-1}\sqrt{at^\mu} n(n-1)(n-2)}{t^{1-2\mu} + 1} - \right. \\ \left. 4\sqrt{at^\mu} \sqrt{at^{\mu/2-1}} F_n j_\mu \frac{(1-\mu)n(n+1)}{n-1} + \frac{n^2(n-1)^2}{(2n-3)} \right] \quad (25)$$

where $G(n, \mu) = [(n+1)(1-\mu)\Gamma(1-\mu)]^{-1} = [(n+1)\Gamma(2-\mu)]^{-1}$

The entire function $E_\mu(t)$ decays in time, but the terms in the brackets are of two types: (1) time – independent and (2) time-dependent and decaying in time. The principle used to minimize $E_\mu(t)$ with respect to the exponent n , focuses the efforts on the time-independent terms depending on n and μ only. From technical point of view (not from mathematical) the elimination of the time-dependent terms, means simply: set $t = 0$ and then solve the equation $E_\mu(n, \mu, t = 0) = 0$, namely:

$$2a^2(1-\mu)F_n^3 j_\mu^3 + \frac{n^2(n-1)^2}{(2n-3)} = 0 \quad (26)$$

The solution of (26), with $F_n = [2n(n-1)]^{1/2}$ and $j_\mu = [(2-\mu)^{-1}\Gamma(2-\mu)]^{1/2}$, gives positive values $n > 1$ as roots. In fact, irrespective of μ , eq. (26) has one trivial solution $n_1 = 0$. Within the range $0 < \mu < 0.7$, eq (26) has three real roots: $n_1 = 0$, $n_2 > 1$ and $n_3 < 0$. In the range $0.7 < \mu < 0.9$, the roots are 5: $n_1 = 0$, $n_2 > 1$ and $n_3 < 0$ and two complex, n_4 and n_5 . The only realistic for any μ is $n = n_2 > 1$ following the basic assumption of the integral profile.

Table 1. Values of the optimal exponent and the fractional correction factor j_μ as function of the fractional order μ

Fractional order, μ	Optimal exponent, n	Fractional correction factor, j_μ
0.1	1.480	0.711
0.2	1.478	0.719
0.3	1.477	0.731
0.4	1.472	0.768
0.5	1.472	0.768
0.6	1.469	0.796
0.7	1.465	0.830
0.8	1.456	0.874
0.9	1.434	0.929

The values of the exponent and the j_μ factor as various μ are summarized in tab. 1. It is obvious, that decrease in μ augments the exponent n and reduces the correction factor j_μ . The latter physically implies: the penetration depth decreases as the fractional order is decreased, and *vice versa*. In the context of the optimal exponent of the integral profile, we have to mention that in the case of normal diffusion, with the same boundary problem, the value is $n \approx 2.235$ [35, 36]. All calculations (from eq. 3 to eq. 26) were performed by Maple 13.

Note 1. The approach in determination of the optimal exponent has only one goal: to find a value that minimize the average-squared error in the equation domain. The expression of (25) shows that probably the exponent is a function of the time, *i. e.* $n = n(t)$ because $E(t)$. However, this draws new problems, which are beyond the scope of the present work.

Note 2. The concept of the penetration depths is valid up to the moment when $\delta(t) = R$. Then, the profile becomes simpler, *i. e.* $\Theta_a R = (1 - r/R)^{n_R}$ and the new exponent n_R should be defined through the fractional heat-balance integral, since the new profile should satisfy it. However, this envisages a new problem beyond the scope of the present work.

Fractional Fourier number and results thereof

The dimensionless time of a normal diffusion in a semi-infinite medium can be expressed as $t/(x^2/a)$, where $t_{0(1)} = r^2/a$ is the time scale. Then, the ratio $t/(r^2/a) = t/t_{0(1)}$ defines the Fourier number. Hence, the approximation profile for the normal diffusion can be expressed as $\Theta(r, t) = [1 - (\text{Fo} F_n)^{-1}]^n$, where, the $\text{Fo}^{-1} = r/(at)^{1/2}$. Subsequently, in the context of the fractional diffusion the ratio $t/t_{0(\mu)} = \text{Fo}_\mu$ defines the fractional Fourier number. The time scale $t_{0(\mu)}$ can be easily defined taking into account that ratio $\eta = r/(a_\mu t^\mu)^{1/2}$ is dimensionless; from $r/(a_\mu t^\mu)^{1/2} = 1$, it follows that $t_{0(\mu)} = (r^2/a_\mu)^{1/\mu}$; then, we get $\text{Fo}_\mu = t/(r^2/a_\mu)^{1/\mu}$. Rearranging Fo_μ as $(\text{Fo}_\mu)^{\mu/2} = (t^\mu a_\mu)^{1/2}/r = 1/\eta$, the approximate profile can be expressed as:

$$\Theta_a(r, t) = \left[1 - \left(\sqrt{(\text{Fo}_\mu)^\mu F_n j_\mu} \right)^{-1} \right]^{n_\mu} \quad (27)$$

The profile (27) contains only one independent variable Fo_μ . The j_μ factor in the denominator allows expressing its contribution to subdiffusion as $(\text{Fo}_\mu)^{\mu/2} j_\mu = (at^\mu/r_\mu^2)^{1/2} \Rightarrow \text{Fo}_\mu^* = t/r_\mu^2/a$ that, in fact, is a new definition of the fractional Fourier number with a length scale $r_\mu = r/\Pi(2 - \mu)$; where $\Pi(2 - \mu) = \Gamma(2 - \mu)/(2 - \mu)$; is the Gauss *Pi* function. From a physical point of view, this means changes in the characteristic length scale which varies from x at $\mu = 1$ to x_μ at $\mu < 1$. The latter implies a medium with internal length scale $r_\mu < \langle r^2 \rangle^{1/\mu}$. Hence, the profile becomes unified for both the normal diffusion and the sub-diffusion:

$$\Theta_a(r, t) = \left[1 - \frac{1}{\sqrt{\text{Fo}_\mu^* F_n j_\mu}} \right]^{n_\mu} \quad \text{or} \quad \Theta_a(r, t) = \left[1 - \frac{r}{R \sqrt{\text{Fo}_{\mu R}^* F_n j_\mu}} \right]^{n_\mu} \quad (28a,b)$$

The fractional Fourier number Fo_μ uses as a length scale the co-ordinate $0 < x < \delta$ since the medium is unsaturated and there no exists a natural length scale, then the profiles is (23a). If the time scale is defined as $\tau_R = (a/R^2)^{1/\mu}$, then the fractional Fourier number is $\text{Fo}_\mu = t/\tau_R$; The dimensionless parameter τ_1 in eq. (11) is in fact, $\text{Fo}_\mu = t/\tau_R$ since the problem of Qui and Liu [27] considers a fractional diffusion across already saturated medium. Then, considering the problem at issue and $(\text{Fo}_\mu)^{\mu/2} = [(t^\mu a)^{1/2}/R]R/r = (\text{Fo}_\mu)^{\mu/2} = \text{Fo}_{\mu R}^{\mu/2} R/r$ the profile can be expressed in the form (28b).

Moments of the distribution

Equation (20b) gives the dimensionless concentration of the diffusion matter (heat) at any location r as function of the time t . The normalized p^{th} moment of the distribution is:

$$\langle r^p \rangle = \frac{\int_0^R \Theta(r, t) r^p 4\pi r^2 dr}{\int_0^R \Theta(r, t) 4\pi r^2 dr} \quad (29)$$

and can be evaluated at any value of p .

The total amount diffused

The normalized total amount diffused up to time t is the zeroth moment ($p = 0$)

$$\frac{M_t}{M_\infty} = \frac{\int_0^\delta \Theta_a[r, \delta(t)] 4\pi r^2 dr}{\int_0^R \Theta_a(R_{t \rightarrow \infty}) 4\pi r^2 dr} = \frac{4\pi \delta^3}{4\pi \left(\frac{R^3}{3}\right)} 2[(n_\mu + 1)(n_\eta + 2)(n_\mu + 3)]^{-1} = \quad (30)$$

Further, using (21) we may express M_t/M_∞ in three distinct forms, namely:

$$\frac{M_t}{M_\infty} = 6 \frac{(a_\mu t^\mu)^{3/2}}{R^3} \Phi(n_\mu, \mu) \quad \frac{M_t}{M_\infty} = 6 \frac{1}{\eta_R^3} \Phi(n_\mu, \mu) \quad \frac{M_t}{M_\infty} = 6\sqrt{\beta^3} \Phi(n_\mu, \mu) \quad (31a,b,c)$$

$$\text{where } \Phi(n_\mu, \mu) = \frac{(F_n j_\mu)^3}{(n_\mu + 1)(n_\eta + 2)(n_\mu + 3)}, \quad \eta_R = \frac{R}{\sqrt{a_\mu t^\mu}}, \quad \beta = \frac{a_\mu t^\mu}{R^2} = \frac{1}{\eta_R^2} \quad (32a,b,c)$$

The parameter $\beta = (a_\mu t^\mu / R^2) = 1/\eta_R^2$ (used in [14]) is the fractional Fourier number Fo_{uR} defined above. The increase of the accumulated mass with the time through the expressions (31a) and (31c) is obvious. The form (31b) is also valid, because η is inversely proportional to the time. The finite time t_∞ is defined by the ratio $(\delta/R) = 1$ that gives: $(a_\mu t_\infty^\mu)^{1/2} F_n j_\mu = R \Rightarrow t_\infty^\mu = [R / (a_\mu F_n j_\mu)^{2/\mu}]$. Hence, the lower limit η_∞ is defined as $\eta_\infty = R / (a_\mu t_\infty^\mu)^{1/2}$; $\eta_\infty \leq \eta < \infty$, where the upper limit corresponds to $t = 0$. Thus, the upper limit of the fractional Fourier number is $(Fo_{uR})_\infty = \beta_\infty = (1/\eta_\infty)^2 = (a_\mu t_\infty^\mu)/R^2$. The introduction of η , η_R , and β allows the approximate distribution to be expressed in forms equivalent to eq. (28a) and eq. (28b):

$$\Theta_a(r, t) = \left[1 - \left(\frac{r}{R} \right) \left(\frac{\eta}{F_n j_\mu} \right) \right]^{n_\eta} = \left[1 - \left(\frac{r}{R} \right) \left(\frac{1}{F_n j_\mu \sqrt{\beta}} \right) \right]^{n_\eta} \quad (33a,b)$$

Mean-square displacement

The numerator for the expression for the second moment in eq. (29) is:

$$\langle r^2 \rangle_{\text{num}} = \int_0^\delta \Theta_a[r, \delta(t)] r^2 4\pi r^2 dr \Rightarrow \langle r^2 \rangle_{\text{num}} = 4\pi \frac{6\delta^4}{(n_\mu + 1)(n_\eta + 2)(n_\mu + 3)(n_\mu + 4)} \equiv t^{2\mu} \quad (34a,b)$$

Hence, the means square displacement in radial direction does not exhibit proportionality to t^μ as in the classical 1-D case. If the sphere is completely saturated, i. e. $\delta = R$, then $\langle r^2 \rangle \equiv 4\pi R^4 t^{2\mu}$.

Numerical experiments

The exponent of the approximate distribution

The numerical data about n_μ (see tab. 1) were plotted against of the fractional order μ (see fig. 1). The nonlinear regression analysis (by Origin 6.0) yields the best correlation by the Gauss distribution, namely:

$$n_\mu \approx n_{\mu 0} + \frac{A}{w} \sqrt{\frac{2}{\pi}} \exp \left[\frac{(n_\mu - n_{\mu c})^2}{w^2} \right] \Rightarrow n_\mu \approx 1.256 + 0.224 \exp \left[\frac{(n_\mu - 0.264)^2}{4.303} \right] \quad (35a)$$

$$\text{with } n_{\mu 0} = 1.256, n_{\mu c} = 0.264, w = 2.074, A = 0.583, \chi^2 = 0.00003, R_{res}^2 = 0.91293 \quad (35b)$$

However, there are two sub-sections of the plot where the relationship $n_\mu = f(\mu)$ exhibits almost linear behaviour: the straight asymptotes are crossing in the range $0.65 < \mu < 0.75$. The asymptotes were approximated by: 1st asymptote ($0.1 < \mu < 0.7$), $n_\mu \approx 1.483 - 0.023 \mu$ and 2nd asymptote ($0.7 < \mu < 0.9$), $n_\mu = 1.57 - 0.156 \mu$. It is worth nothing, that these numerical results should be considered as purely empirical data obtained through a numerical experiments and absence of any theoretical relationship between the profile exponent n_μ and fractional order μ .

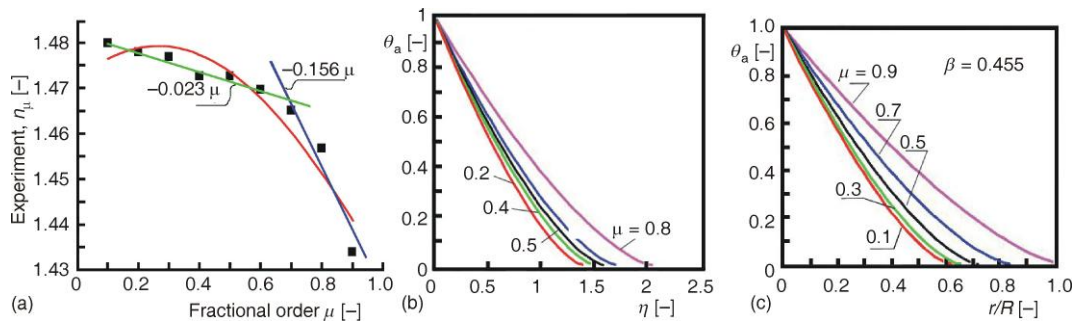


Figure 1. First outcomes of the approximate solution: (a) relationship between the optimal exponent of the approximate profile and the fractional order of the subdiffusion equation; (b) approximate profile generated distributions as a function of the similarity variable η at various values of μ ; (c) radial approximate profiles at various of μ and the Fourier number a global parameter

Time evolution of the distribution

The time-fractional subdiffusion equations generate distributions which in the present case are approximated by the parabolic profile (6). With the developed relationships about $\delta(t)$ and n_μ , some examples are shown in fig. 1b. The distributions are expressed as unique functions of the similarity variable $\eta = r/(a_\mu t^\mu)^{1/2}$ (see eq. 21).

The radial distributions of the concentration

Equations (33a,b) give the radial distribution as function of r/R and β as a parameter (i. e. at different times). Plots various values of μ and the fractional Fourier number are shown in fig. 1c.

Penetration depth $\delta(t)$

The normalized penetration depth $\delta(t)/R = [(a_\mu t^\mu)^{1/2}/R] F_n j_\mu = \beta^{1/2} F_n j_\mu$ depends only on the fractional Fourier number β . The plots in fig. 2 reveals that decrease in the fractional order μ decelerate the motion of the matter in depth of the medium that is a physically reasonable result. Three stages are illustrated: short-times (fig. 2a), medium-times (fig. 2b)

and large-times (fig. 2c). The figures are quite illustrative showing simultaneously the time-dependent front propagation and the retardation of the diffusion process when the fractional order μ decreases.

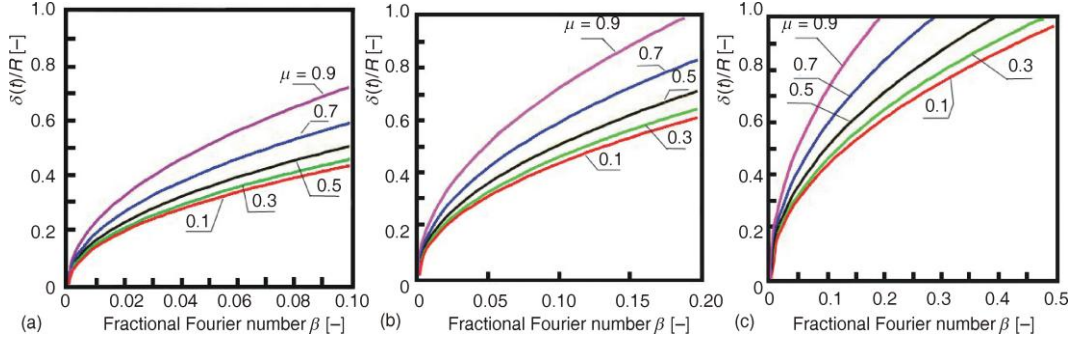


Figure 2. Time-evolutions of the penetration depth: (a) short times; (b) medium times; (c) large times

The mean square displacement

Equation (34b) can be expressed as the ratio $\langle r^2 \rangle / R^2$ (see eq. 31, eq. 32) and the consequent discussion in section 8.1, namely:

$$\frac{\langle r^2 \rangle}{R^4} \equiv \frac{\delta^4}{R^4} = \Omega(\mu) \left(\frac{a_\mu t^\mu}{R^2} \right)^2 \equiv \beta^2 \equiv \frac{1}{\eta_R^2} \equiv (\text{Fo}_{\mu R})^2 \quad (36)$$

where $\Omega(\mu) = 24\pi(F_n j_\mu)^4 [(n_\mu + 1)(n_\mu + 2)(n_\mu + 3)(n_\mu + 4)]^{-1}$

The plot of the second moment as a function of β is shown in fig. 3a,b for short and large-time stages. These results confirm the solution in [14] that the curves depends only on the dimensionless parameter β (the fractional Fourier number). Moreover, this is a performance of the universality exhibited by the solution since the same dependence is exhibited by the normal diffusion at $\mu = 1$. Additionally, the second moment growth in time is a specific for diverged flow from the sphere center to the surface. The opposite behavior was demonstrated in [14] when an inward radial diffusion (from R_2 to R_1 , $R_2 > R_1$) problem was solved.

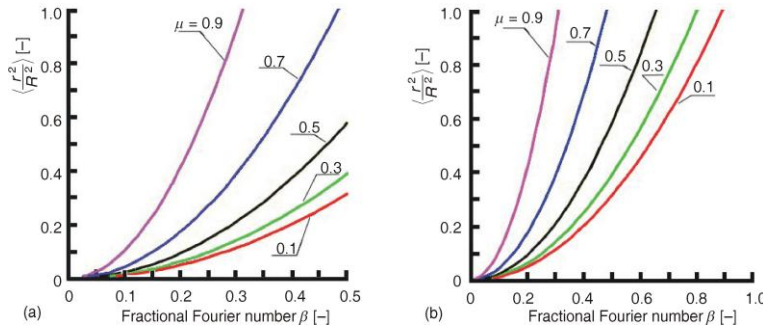


Figure 3. Mean-square displacement as a function of the Fourier number: (a) short times; (b) large times

The total amount diffused

The dimensionless total amount diffused (see eqs.(31a,b,c)) is plotted as a function of β (dimensionless time) in Fig. 4a,b. In fact, it repeats the behaviour of the second moment due the inherent relationship.

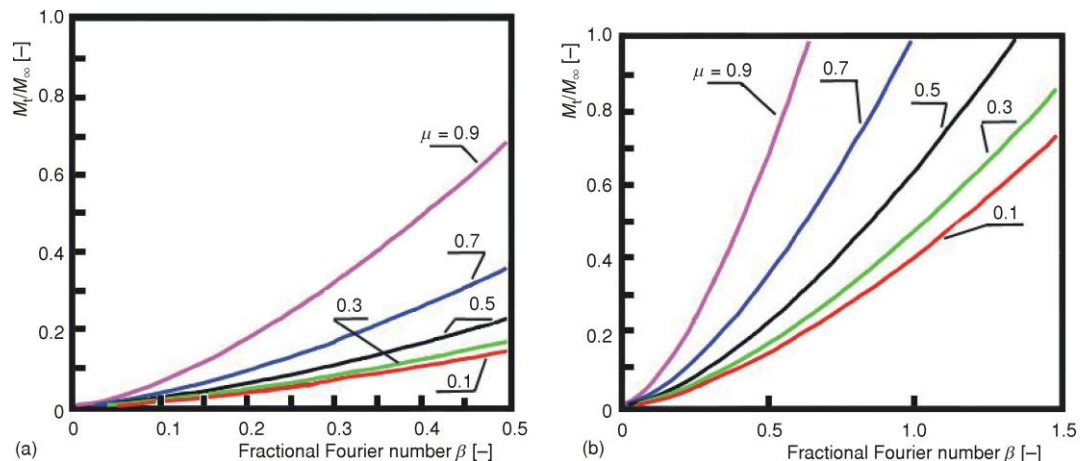


Figure 4. Total amount diffused (dimensionless) as a function of β ; (a) short times, (b) large times

Discussion

The problems were discussed parallel to the development of the integral solution, but we will briefly outline the main points. The method developed was successfully applied for years to transient (Fikian) diffusion and Stefan problems. The developed solution is the first attempt to apply the heat-balance integral method (a moment method with a weight function equal to 1) to a subdiffusion equation. The penetration layer has a physical meaning because either the heat or the mass diffusion controlled by the sub-diffusion equation propagates slowly into the medium. The rate of this propagation depends on the degree of deviation from the normal (Fikian) diffusion expressed through the fractional order μ . The fractional Fourier number (or the parameter β) controls the diffusion process as a unique time-dependent parameter.

An interesting numerical results obtained is the relationship between the exponent of the approximate profile and the fractional order μ . The optimal exponent was defined through the classical mean-square error approach that leads to cumbersome expressions, as in the normal diffusion problems, too. This raises a problem for of more simple ways in finding the exponent and minimization of the approximation error, as well. In this context, the purely physical approach in the minimization of the approximation error and determination of the optimal exponent could be replaced by more strong mathematical operations.

The solution ended at the moment when the front of the penetration depth reached the outer sphere surface. The diffusion then continues, but now with R instead δ as a length scale. The solution in the same manner is possible but envisages a problem beyond the scope of the present work.

The simulated distributions and radial profiles are physically adequate since they clearly demonstrate how the fractional order decelerates ($\mu \rightarrow 0.1$) or forces ($\mu \rightarrow 0.9$) the propagation of the diffusion matter.

Conclusions

Integral solution to a radial time-fractional subdiffusion from point source in sphere was developed. The fractional heat-balance integral allows easily obtaining an approximate solution without shifting from Riemann-Liouville to Caputo derivatives because the step with the Laplace transform is avoided.

The solution was demonstrated through a parabolic profile with an unspecified exponent as a more general expression of the polynomial profiles used in the classical heat-balance integral method. This profile needs the exponents to be defined additionally and through the mean-square error approach the solution combines both the moment method (the heat-balance integral) and the condition the domain equation to be satisfied, too. The numerical results in the definition of the profile exponent reveal a strong relationship to the fractional order μ .

The numerically simulated results are adequate and show the effect of the deviation from the normal diffusion on the solution generated distributions, radial profiles, the time-evolution of both the penetration layer and the total amount diffused.

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