

General Similarity Solution of the Fragmentation Kinetics Equation

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Z. Naturforsch. **59a**, 309–315 (2004); received October 26, 2003

In this article we have discussed a new application of Lie's similarity method on the integro-differential fragmentation equation. A wide variety of the similarity solutions of the fragmentation equation has been obtained. Some of them are compared with those obtained by other authors.

Key words: Similarity Solution; Similarity Reduction; Fragmentation Equation; Fox Function.

1. Introduction

Fragmentation results from a variety of physical processes, such as erosion, polymer degradation, grinding, oxidation and dissolution. The authors of [1–3] determined the distribution function by statistical methods considering random scission processes where all bonds break with equal probability [2]. Later Saito [4] and Jellinek et al. [5] studied continuous and discrete fragmentation processes, respectively. The continuous model introduced by Saito has wide applications in physics, see for instance Peterson [6].

However, a linear fragmentation rate equation describing polymer breakup due to degradation of bonds has received considerable attention [7–10]. Besides, a nonlinear rate equation describing fragmentation due to repeated collisions between particles has been developed [10]. These rate equations are similar in spirit to the well-known nonlinear Smoluchowski equation for coagulation [11–12]. Even though the spatial homogeneity inherent in rate equations is sometimes obeyed only approximately in experiments, rate equations have nevertheless added considerable insight to the overall understanding of fragmentation. Compared with numerical simulations [13–15], the advantage of the rate equation approach is its generality: general forms for fragmentation rates and daughter distribution allow for solutions which span a spectrum of particle morphologies, external conditions, and fragmentation processes, whereas numerical simulations typically require specific particle morphologies and external conditions.

Much of the theoretical work is based on the description of fragmentation by a system of linear rate equations in the discrete forms which are suitable for numerical analysis. For an analytical treatment of fragmentation the continuous models are more appropriate. The continuous models are typically represented by a linear integro-differential balance equation. In a generalized nonlinear model Cheng et al. [10] proposed a fragmentation process caused by repeated collisions between clusters. Amemiya [16] introduced on the other hand an inhomogeneity by assuming bonds of different breaking probability dispersed throughout the system. The dependence of the scission rate on the size of the chains was considered by Basedow et al. [17] and Ballauf et al. [18] in theoretical and numerical work.

Following the work of Ziff et al. [7], the fragmentation rate equation with homogenous forces of the break up kernel can be described by the following integro-differential equation

$$\frac{\partial n(x,t)}{\partial t} = -n(x,t) \int_0^x F(y, x-y) dy + 2 \int_x^\infty n(y,t) F(x, y-x) dy, \quad (1)$$

where $n(x,t)$ is the number of chains of continuous length x at time t and the kernel $F(x,y)$ gives the rate that a segment breaks up into two parts of lengths x and y . Different forms of the break up kernel lead to different classes of the kinetic Eq. (1), for details

see [7]. One of these classes is

$$\frac{\partial u(x,t)}{\partial t} + x^{\gamma+1}u(x,t) - 2 \int_x^\infty y^\gamma u(y,t) dy = 0, \quad (2)$$

where

$$F(x,y) = (x+y)^\gamma, \quad (3)$$

$$F(\lambda x, \lambda y) = \lambda^\gamma F(x+y), \quad u(x,t) = n(x,t). \quad (4)$$

The partial differential equation corresponding to (2) is obtained by differentiating (2) with respect to x

$$u_{xt}(x,t) = -x^\gamma((1+\gamma)+2)u(x,t) - x^{1+\gamma}u_x(x,t), \quad (5)$$

where the exponent γ determines the degree of homogeneity of this model.

Normally Lie's technique is successfully applied to partial differential equations such as (5). In spite of the growing interest in the application of Lie's method of solving differential equations, the number of cases where Lie's method has been applied to integro-differential equations is very small.

So, the motivation of this paper is to show first how one can use Lie's group approach for integro-differential equations such as the fragmentation equation (2). In addition, we also aim to obtain the general similarity solution and classify the obtained solutions in terms of the Lie group parameters.

2. Lie Analysis

We consider the one-parameter (ε) group of infinitesimal transformations

$$\begin{aligned} x^* &= x + \varepsilon\xi(x,t,u) + 0(\varepsilon^2), \\ t^* &= t + \varepsilon T(x,t,u) + 0(\varepsilon^2), \\ u^* &= u + \varepsilon\eta(x,t,u) + 0(\varepsilon^2), \\ u_{t^*}^* &= u_t + \varepsilon[\eta_t] + 0(\varepsilon^2), \\ \int_{x^*}^\infty y^\gamma u^* dy &= \int_x^\infty y^\gamma u dy + \varepsilon[\Delta I], \end{aligned} \quad (6)$$

where the infinitesimal $[\eta_t]$ is given by

$$[\eta_t] = \eta_t + (\eta_u - T_t)u_t - \xi_t u_x - T_u u_t^2 - \xi_u u_x u_t. \quad (7)$$

In addition, it can be proved that

$$[\Delta I] = -\xi x^\gamma u \quad (8)$$

$$+ \int_x^\infty \left[n\xi y^{\gamma-1}u + y^\gamma\eta + y^\gamma u \left[\frac{\partial \xi}{\partial y} + \frac{\partial \xi}{\partial u} \frac{\partial u}{\partial y} \right] \right] dy.$$

In the infinitesimal representation, an equation corresponding to the transformation (6) can be written as

$$\chi = \xi \frac{\partial}{\partial x} + T \frac{\partial}{\partial t} + \eta \frac{\partial}{\partial u} + [\eta_t] \frac{\partial}{\partial u_t} + [\Delta I] \frac{\partial}{\partial \int y^\gamma u dy}, \quad (9)$$

where T, ξ, η are all functions of t, x, u which can be determined using the invariant Lie group approach [19]. The infinitesimal criteria for the invariance of (2) under the group (6) is given by

$$\chi H = \lambda(x,t,u)H, \quad (10)$$

where

$$H\left(x,t,u,u_t \int_x^\infty y^\gamma u dy\right) = u_t + (x^{\gamma+1})u - \int_x^\infty y^\gamma u dy, \quad (11)$$

and $\lambda(x,t,u)$ is an arbitrary function to be determined. By means of (9), (10) and (11), the determining equations for T, ξ, η and λ are

$$\begin{aligned} \frac{\partial \eta}{\partial u} - \frac{\partial T}{\partial t} &= \lambda(x,t,u), \quad \frac{\partial \xi}{\partial t} = \frac{\partial \xi}{\partial u} = 0, \\ \frac{\partial T}{\partial x} &= \frac{\partial T}{\partial u} = 0, \quad \frac{\partial^2 \eta}{\partial u^2} = 0, \\ \frac{\partial \eta}{\partial t} + x^{\gamma+1}\eta + (1+\gamma)x^\gamma\xi u &= \lambda(x,t,u)x^{\gamma+1}u, \\ \int_x^\infty \left[\gamma y^{\gamma+1}\xi u + y^\gamma\eta + y^\gamma u \left[\frac{\partial \xi}{\partial y} + \frac{\partial \xi}{\partial u} \frac{\partial u}{\partial y} \right] \right] dy \\ &= \lambda(x,t,u) \int_x^\infty y^\gamma u dy. \end{aligned} \quad (12)$$

After considerable algebra and many integrations, the set of equations (12) yields the most general Lie group symmetries

$$\begin{aligned} T &= a_0 t + a_1, \quad \xi = \frac{a_2}{(\gamma+1)}x^{-\gamma} - \frac{a_0}{1+\gamma}x, \\ \eta &= (a_3 - a_2 t)u + \phi(x,t), \end{aligned} \quad (13)$$

where $a_i (i = 0, 1, 2, 3)$ are constants and $\phi(x,t)$ has to solve the original equation (2). Thus the problem of finding the full Lie symmetries of (12) involves finding general solutions of (2). This is an impossible task, therefore we choose $\phi(x,t) = 0$ with no loss in generality. Now, it is clear that the most extended Lie group of transformations admitted by the partial integro differential equation (2) depends on four arbitrary group parameters, a_0, a_1, a_2, a_3 . The knowledge of the infinitesimal elements T, ξ , and η enables us to determine

Table 1. Similarity forms and reduced dynamic equations of the fragmentation.

Case	Similarity forms	Reduced dynamic equation of aerosols
1	$u = F(s)(a_0t + a_1)^m \exp\left[-\frac{a_2}{a_0}t\right], \quad s = (a_0t + a_1)(a_2 - a_0x^{\gamma+1}),$ $m = \frac{1}{a_0} \left(a_3 + \frac{a_1 a_2}{a_0} \right)$	$a_0 s \frac{dF}{ds} + (a_0 m - \frac{\gamma+1}{a_0} s) F(s) + \frac{2}{a_0} \int_s^\infty F(s') ds' = 0$
2	$u = F(s)(a_0t + a_1)^{a_3/a_0}, \quad s = x(a_0t + a_1)^{1/1+\gamma},$	$\frac{a_0}{1+\gamma} s \frac{dF}{ds} + (a_3 + s^{1+\gamma}) F(s) - 2 \int_s^\infty s'^\gamma F(s') ds' = 0$
3	$u = F(s) \exp\left[\frac{a_3}{a_2} - s\right] x^{1+\gamma}, \quad s = t$	$(1+\gamma) \left(\frac{a_3}{a_2} - s \right) \frac{dF}{ds} + 2F(s) = 0$
4	$u = F(s) e^{\frac{1}{a_1} \left(a_3 t - \frac{a_2}{2} t^2 \right)}, \quad s = \frac{a_2}{a_1} t - x^{\gamma+1}$	$\frac{a_2}{a_1} \frac{dF}{ds} + \left(\frac{a_3}{a_1} - s \right) F(s) + \frac{2}{\gamma+1} \int_s^\infty F(s') ds' = 0$
5	$u = F(s), \quad s = x$	$s^{\gamma+1} F(s) - 2 \int_s^\infty s'^\gamma F(s') ds' = 0$
6	$u = F(s) e^{\frac{a_3}{a_1} t}, \quad s = x$	$\left(\frac{a_3}{a_1} + s^{\gamma+1} \right) F(s) - 2 \int_s^\infty s'^\gamma F(s') ds' = 0$

$\lambda(x, t, u)$ via the first equation in (12). In addition it gives rise to the extended symmetries generated by

$$\begin{aligned} \chi_1 &= \frac{\partial}{\partial t}, \quad \chi_2 = u \frac{\partial}{\partial u}, \quad \chi_3 = t \frac{\partial}{\partial t} - \frac{1}{\gamma+1} x \frac{\partial}{\partial x}, \\ \chi_4 &= \frac{1}{1+\gamma} x^{-\gamma} \frac{\partial}{\partial x} - t u \frac{\partial}{\partial u}. \end{aligned} \quad (14)$$

These four linear independent vector fields determine the symmetries under which the partial integro-differential equation (2) is invariant, and in addition the symmetries that constitute a Lie algebra. The vector fields χ_2 and χ_3 contain the scaling properties of u, t, x , and χ_1 corresponds to a translation in time. The commutation relations of the four vector fields χ_1, χ_2, χ_3 and χ_4 are

$$[\chi_1, \chi_3] = \chi_1, [\chi_1, \chi_4] = \chi_2, [\chi_3, \chi_4] = \chi_4, \quad (15)$$

and the rest equals zero. We can use a combination of these vector fields to classify the type of similarity solutions. One may find the six essential combinations listed in Table 1. These produce the essential types of reduced partial integro-differential fragmentation equations in one new variable s as well as the similar solution $F(s)$.

3. General Similarity Solution

A linear combination of the four vector fields χ_1, χ_2, χ_3 and χ_4 , where the group parameters a_0, a_1, a_2 , and a_3 are all unequal to zero determines

the general similarity solutions of the fragmentation equation. Thus finding the similarity solution associated with the combination $\chi_1 + \chi_2 + \chi_3 + \chi_4$ solves the general problem, and hence the solution of other cases in Table 1 appears to be a special class of the general one. However, integrating the characteristic equation

$$T^{-1} dt = \xi^{-1} dx = \eta^{-1} du, \quad (16)$$

with the group (13), yields the general similarity solution

$$u = F(s)(a_0t + a_1)^m \exp\left[-\frac{a_2}{a_0}t\right], \quad (17)$$

where

$$\begin{aligned} s &= (a_0t + a_1)(a_2 - a_0x^{\gamma+1}), \\ m &= \frac{1}{a_0^2}(a_0a_3 + a_1a_2). \end{aligned} \quad (18)$$

Substitution this similarity solution into (2) results in the following reduced fragmentation equation:

$$a_0 s \frac{dF}{ds} + (a_0 m - \frac{\gamma+1}{a_0} s) F(s) + \frac{2}{a_0} \int_x^\infty F(s') ds' = 0. \quad (19)$$

Use of the substitution

$$g(s) = \int_x^\infty F(s') ds' \quad (20)$$

transforms (19) to the following second order differential equation with variable coefficients

$$s \frac{d^2g}{ds^2} + \left(m - \frac{\gamma+1}{a_0^2} s \right) \frac{dg}{ds} - \frac{2}{a_0} g(s) = 0. \quad (21)$$

Rescaling s by $\zeta = \frac{\gamma+1}{a_0} s$, (21) can be reduced to the standard form of Kummer's equation

$$\zeta = \frac{dg}{d\zeta^2} + (m - \zeta) \frac{dg}{d\zeta} - \frac{2}{\gamma+1} g(\zeta) = 0. \quad (22)$$

The complete solution of (22) can be expressed in terms of the confluent hypergeometric function ${}_1F_1(a, b, \zeta)$ which consists of a convergent series for ζ . However, the solution is (see for instance Kamke [20])

$$g(\zeta) = A_1 {}_1F_1\left(\frac{2}{\gamma+1}, m; \zeta\right) + B_1 \zeta^{1-m} {}_1F_1\left(\frac{2}{\gamma+1} - m + 1, 2 - m; \zeta\right), \quad (23)$$

where ${}_1F_1(a, b, \zeta)$ is given by the series

$${}_1F_1(a, b, \zeta) = 1 + \sum_{r=0}^{\infty} \frac{(a)_r \zeta^r}{(b)_r r}, \quad (24)$$

and $(a)_r$, $(b)_r$ are Pochhammer's symbols define by $(a)_r = \Gamma(a+r)/\Gamma(a)$, $(b)_r = \Gamma(b+r)/\Gamma(b)$. A and B are two arbitrary constants. Inverting the transformation used previously, one can write down the most general similarity solution of the integro-differential fragmentation equation. In addition to the general similarity for the fragmentation equation (2),

we distinguish four particular classes of similarity solutions.

First Class:

This class of similarity solution can be obtained if we put $a_0 = 0$ in (13). With this choice the general similarity solution (17) reduces to

$$u = F(s) \exp \left[\frac{1}{a_1} \left(a_3 t - \frac{a_2}{2} t^2 \right) \right], \\ s = \frac{a_2}{a_1} t - x^{1+\gamma}. \quad (25)$$

This case corresponds to the vector field combination $\chi_1 + \chi_2 + \chi_4$. Inserting the above similarity solution into (2), the reduced fragmentation equation is

$$\frac{a_2}{a_1} + \frac{dF}{ds} + \left(\frac{a_3}{a_4} - s \right) F(s) + \frac{2}{\gamma+1} \int_s^{\infty} F(s') ds' = 0. \quad (26)$$

Via the substitution

$$g(s) = \int_s^{\infty} f(s') ds', \quad (27)$$

the reduced fragmentation equation (26) is transformed to the second order differential equation with variable coefficients

$$\frac{d^2g}{ds^2} + \left(\frac{a_3}{a_2} - \frac{a_1}{a_2} s \right) \frac{dg}{ds} - \frac{2(a_1/a_2)}{1+\gamma} g(s) = 0, \quad (28)$$

whose solution is

$$g(s) = \exp \left[- \frac{s \left[B_1(1+\gamma) - B_2(1+\gamma)s + \sqrt{8(1+\gamma)B_2 + (1+\gamma)(B_1 - B_2s)^2} \right]}{2(1+\gamma)} \right] \cdot \left[c_1 \exp \left[\frac{s \sqrt{8(1+\gamma)B_2 + (1+\gamma)(B_1 - B_2s)^2}}{1+\gamma} \right] + c_2 \right], \quad (29)$$

where $B_1 = a_3/a_2$, $B_2 = a_1/a_2$, c_1 and c_2 are arbitrary constants. Inverting the transformations used previously, one can express the solution in terms of the original coordinates x, t, u . The behavior of $u(x, t)$ versus x for fixed values of time is shown graphically in Figure 1.

It is worth noting that on the one hand if $a_2 = 0$, the similarity solution (25) reduces to

$$u = F(s)t, \quad s = tx^{\gamma+1}, \quad (30)$$

and on the other hand this leads to the solutions discussed previously by McGrady et al. [9] and Corngold

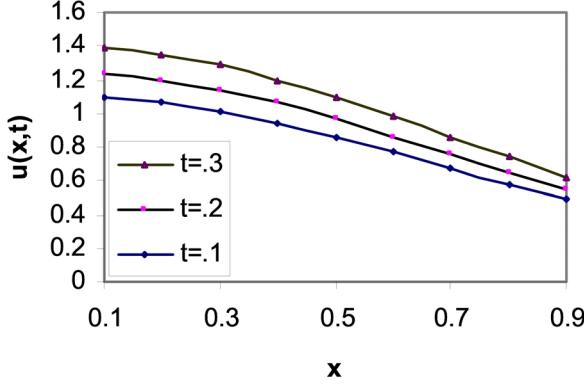


Fig. 1. The behavior of the similarity solution (29) versus x for $t = 0.1, 0.2, 0.3$.

et al. [21]. This case corresponds to the particular case $\chi_2 + \chi_3$. This means that the solutions obtained by [9] and [21] are thus similarity solution corresponding to the particular case $\chi_2 + \chi_3$.

Second Class:

In this case $a_3 = 0$, integrating the characteristic Eq. (16) yields

$$u = F(s) \exp \left[-\frac{c}{2} t^2 \right], \quad (31)$$

$$s = x^{1+\gamma} - ct, \quad c = \frac{a_2}{a_1}.$$

The reduced equation becomes

$$\frac{d^2 g}{ds^2} - \frac{1}{c} s \frac{dg}{ds} - \frac{2}{c(1+\gamma)} g(s) = 0, \quad (32)$$

where $g(s)$ is defined by (27). Using the scaling transformation $\zeta = \sqrt{1/cs}$, (32) transforms to

$$\frac{d^2 g}{d\zeta^2} - \zeta \frac{dg}{d\zeta} - kg(\zeta) = 0, \quad (33)$$

where $k = 2/(1+\gamma)$. The general solution of this ordinary differential equation can be given in terms of a special type of Fox function [22]:

$$g(\zeta) = c_1 H_{23}^{12} \left(-2\zeta^2 \left| \begin{matrix} (0,1) & \left(1 - \frac{1}{2}k, 1 \right) \\ (0,1) & (0,2) & \left(1 - \frac{1}{2}k, 0 \right) \end{matrix} \right. \right) + c_2 \zeta H_{23}^{12} \left(-2\zeta^2 \left| \begin{matrix} (0,1) & \left(\frac{1}{2}(1-k), 1 \right) \\ (0,1) & (-1,2) & \left(\frac{1}{2}(1-k), 0 \right) \end{matrix} \right. \right), \quad (34)$$

or equivalently by Maitland's generalized hypergeometric functions, which are also called Wright functions:

$$g(\zeta) = c_{12} \Psi_3 \left(\begin{matrix} (1,1) & \left(\frac{1}{2}k, 1 \right) \\ (1,2) & \left(\frac{1}{2}k, 0 \right) \end{matrix} ; 2\zeta^2 \right) + c_2 \zeta_2 \Psi_3 \left(\begin{matrix} (1,1) & \left(\frac{1}{2}(k+1), 1 \right) \\ (2,2) & \left(\frac{1}{2}(k+1), 0 \right) \end{matrix} ; 2\zeta^2 \right). \quad (35)$$

The Wright function, see [23], are defined as

$${}_p\Psi_q \left(\begin{matrix} (a_1, \alpha_1) \dots (a_p, \alpha_q) \\ (b_1, \beta_1) \dots (b_q, \beta_p) \end{matrix} ; \zeta \right) = \sum_{k=0}^{\infty} \frac{\prod_{j=1}^p \Gamma(a_j + \alpha_j k)}{\prod_{j=1}^q \Gamma(b_j + \beta_j k)} \frac{(-\zeta)^k}{k}.$$

Third Class:

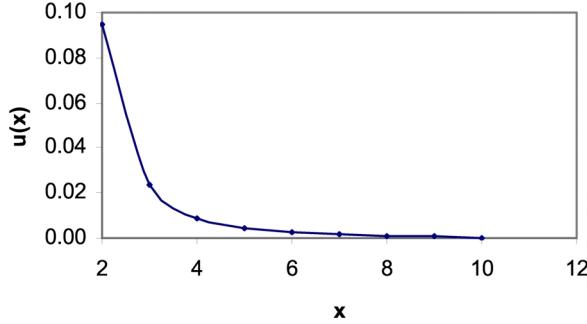
A further similarity solution can be generated by the vector field $\chi_1 + \chi_2$, which corresponds to a trans-

lational symmetry in time and scaling of the dependent variable u . Solving the corresponding characteristic Eq. (16) yields

$$u = F(s) \exp \left[\frac{a_3}{a_1} t \right], \quad s = x. \quad (36)$$

With the similarity representation (6)–(10), the fragmentation equation (2) reduces to the equation

$$\left(\frac{a_3}{a_2} + s^{1+\gamma} \right) F(s) - 2 \int_s^{\infty} s'^{\gamma} F(s') ds' = 0. \quad (37)$$

Fig. 2. The behavior of the similarity solution (42) versus x .

By means of the transformation $\zeta = s^{1+\gamma}/(1+\gamma)$, (37) becomes

$$\left(\frac{a_3}{a_2} + (1+\gamma)\zeta\right)F(\zeta) - 2 \int_{\zeta}^{\infty} F(\zeta') d\zeta' = 0. \quad (38)$$

Employing (27), this integral equation can be transformed to

$$\left(\frac{a_3}{a_2} + (1+\gamma)\zeta\right) \frac{dg}{d\zeta} + 2g = 0, \quad (39)$$

which yields

$$g = g_0 \left(\frac{a_3}{a_2} + (1+\gamma)\zeta\right)^{-\frac{2}{1+\gamma}}, \quad (40)$$

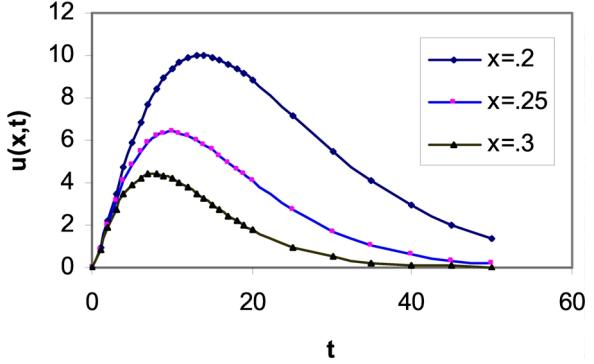
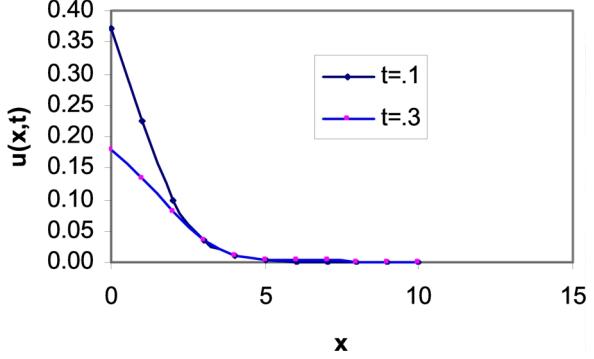
where g_0 is a constant. By means of the transformation (27), with (36) and (40) one can write down an expression for u in terms of x and t :

$$u = g_0 \left(\frac{a_3}{a_2} + (1+\gamma)x^{1+\gamma}\right)^{-\frac{3+\gamma}{1+\gamma}} \exp\left[\frac{a_3}{a_1}t\right]. \quad (41)$$

Since the steady solution of the fragmentation process is very important from the practical point of view, we are interested in finding such a solution. Considering $a_3 = 0$, the stationary solution of the fragmentation equation is

$$u(x) = g_0 x^{-(3+\gamma)}. \quad (42)$$

We conclude that, when $a_3 = 0$, this stationary solution of the fragmentation equation (2) is a similarity solution corresponding to time translation invariance. This type of solution is shown graphically in Figure 2.

Fig. 3. The behavior of the similarity solution (47) versus t for $x = 0.2, 0.25, 0.3$.Fig. 4. The behavior of the similarity solution (47) versus x for $t = 0.1, 0.3$.

Fourth Class:

This case is related to $a_0 = a_1 = 0$. The corresponding characteristic equation in this case is

$$\frac{dt}{0} = \frac{(1+\gamma)dx}{x^{-\gamma}} = \frac{du}{(a_3 - a_2 t)u}. \quad (43)$$

Integrating the above equation yields the similarity transformation

$$s = t, \quad u = F(s) \exp\left[\frac{a_3}{a_2} - s\right] x^{1+\gamma}. \quad (44)$$

Inserting the similarity transformation (44) into (2), one can see that the function $F(s)$ should satisfy the reduced equation

$$(1+\gamma) \left(\frac{a_3}{a_2} - s\right) \frac{dF}{ds} + 2F(s) = 0, \quad (45)$$

which admits the solution

$$F(s) = F_0 \left(\frac{a_3}{a_2} - s\right)^{\frac{2}{1+\gamma}}. \quad (46)$$

With the help of (46), the similarity solution (44) in terms of the original coordinate x, t becomes

$$u = F_0 \left(\frac{a_3}{a_2} - t \right)^{\frac{2}{1+\gamma}} \exp \left(\left[\frac{a_3}{a_2} - t \right] x^{1+\gamma} \right). \quad (47)$$

The behavior of this solution against t and x is shown graphically in Figures 3 and 4.

Conclusions

It can be concluded that, based on using the Lie group approach for the integro-differential equation, in addition to the general similarity solution, wide classes

of similarity solutions have been obtained. Depending on the Lie group parameters, it is shown here that some types of similarity solutions for the fragmentation equation (2) are mapped to well known functions such as Kummer's and Fox functions. Moreover, the obtained solutions are compared with those obtained previously by many authors, and it is shown that some of these solutions can be constructed as particular cases from our solutions. Three types of the obtained solutions are shown graphically.

Finally, the Lie group method represents one of the most powerful analytical techniques for solving either differential or integro-differential equations.

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