IOSR Journal of Mathematics (IOSR-JM)
e-ISSN: 2278-0661,p-ISSN: 2278-8727, Volume 20, Issue 4, Ser. 2 (July. – August. 2024), PP 15-18
www.iosrjournals.org

Inverse Problem In Population Balance Equation For Breakage Process Using Similarity

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Abstract:
Solution of inverse population breakage equation is the process of finding the breakage rate and daughter particle distribution from given population density function. This paper describes the similarity behavior of daughter particle distribution. For different values of cumulative volume fraction $F(x,t)$, $\ln t$ versus $\ln x$ curves collapse into a single curve by translation parallel to the $\ln t$ axis. This indicates for similarity behavior.
***Keywords**: Integro-differential equation, Breakage equation, Population density function, Similarity transformation, Kernel, Self-similarity*

Date of Submission: 21-07-2024 Date of Acceptance: 31-07-2024

I. Introduction

Aggregation and breakage process are the main kind of population balance equation. Two or more particles are combined to form a large particle for aggregation whereas a particle breaks into two or more particles in breakage. In this paper, we will consider the breakage process. A population balance analysis of breakage process was first introduced by Valentas and Amundson [5] in 1966 in dispersed phase systems in the chemical engineering literature. In this process, a parent particle undergoes erosion and give daughter particles. Mathematical model of breakage is

$$\frac{\partial f(x,t)}{\partial t} = \int_x^\infty b(x')\, w(x,x')\, f(x',t)\, dx' - b(x) f(x,t)$$
(1)

where $f(x,t)$ is population density function and $b(x)$ is breakage frequency and $w(x,x')$ is breakage distribution function.

II. Preliminaries

Definition 2.1. Self-similar solution

Self-similar solution identifies invariant domains in the space of the independent variables along which the solution remains the same or contains a part that is the same. Self-similar solution of equation (1) is of the form [8]

$$f(x,t) = h_1(t)\, \psi(z), \qquad z = h_2(t)\, x$$
(2)

This solution contains the part $\psi(z)$, which remains the same along the invariant on the (x,t) plane defined by $z = c$ (a constant).

Definition 2.2 Cumulative volume fraction

Cumulative volume fraction is defined as

$$F(x,t) = \frac{1}{\mu_1} \int_0^x x'\, f(x',t)\, dx'$$
(3)

where μ_1 represents the mass density of particles and is given by

$$\mu_1(t) = \int_0^\infty x\, f(x,t)\, dx$$
(4)

Using self-similar form (1), cumulative volume fraction changes to the form

$$F(x,t) = \frac{\int_0^z z'\,\psi(z')\,dz'}{\int_0^\infty z'\,\psi(z')\,dz'} \equiv \varphi(z)$$
(5)

which is itself time-invariant along $z = c$, i.e., it has a self-similar form.

Thus, similarity transformation for $F(x,t)$ is easy as compare to $f(x,t)$. So, equation (1) is transformed in cumulative volume fraction as

$$\frac{\partial F(x,t)}{\partial t} = \int_x^\infty b(x')\,G(x,x')\,\frac{\partial F(x',t)}{\partial x'}\,dx'$$
(6)

where

$$G(x,x') = \frac{1}{x'}\int_0^x y\,w(y,x')\,dy$$
(7)

which represents cumulative volume fraction of particle of size less than or equal to x formed from the breakage of particle of size x'.

According to Filippov [4] and Ramakrishna [1], for the power law breakage rate i.e. $b(x) = k\,x^{\alpha}$ and for similar daughter particle distribution i.e. $G(x,x') = g\left(\frac{x}{x'}\right)$, equation (6) shows the similarity transformation of the type $z = x^{\alpha}\,t$.

The daughter particle distribution function in more general form is considered by Narsimhan et al. [7] as follows:

$$G(x,x') = g\left(\frac{b(x)}{b(x')}\right)$$
(8)

Here, g is a cumulative distribution function with respect to its argument in the interval $[0,1]$ with $g(1) = 1$.

By using the transformation, $F(x,t) = \varphi(z),\ z = b(x)\,t$ and using equation (8), equation (6) transforms into the following equation:

$$z\,\varphi'(z) = \int_z^\infty g\left(\frac{z}{z'}\right)\,z'\,\varphi(z')\,dz'$$
(9)

Inverse problem formulation

According to Sathyagal et al. [3], the relation between t and x at constant z can be obtained from the data of $F(x,t)$ versus x at various t as the self-similarity implies that the cumulative fraction $F(x,t)$ is invariant on $z = b(x)\,t$. Thus, we have

$$\left(\frac{\partial x)}{\partial t}\right)_F = \left(\frac{\partial x)}{\partial t}\right)_z$$

which on simplification gives,

$$\left(\frac{\partial\,ln\,t}{\partial\,ln\,x}\right)_F = -\frac{d\,ln\,b(x)}{d\,ln\,x}$$
(10)

Equation (10) shows that slope of the $ln\,t$ versus $ln\,x$ curves at various F depends only on x. So, these curves must merge into a single curve by translation of the curve along $ln\,t$ co-ordinates. This single curve must have range of x from x_0 to x_{max}.

On integrating equation (10) from reference size x_0 to x, we get

$$b(x) = \beta\, exp\left[-\int_{ln\,x_0}^{ln\,x} \left(\frac{\partial\, ln\, t}{\partial\, ln\, x}\right)_F\, d\, ln\, x\right]$$
(11)

where β is the breakage rate of the particle of size x_0.

Due to lack of information about exact $b(x)$ and similarity variable z, we define a new similarity variable as,

$$\xi = \frac{b(x)\, t}{\beta} = exp\left[-\int_{ln\,x_0}^{ln\,x} \left(\frac{\partial\, ln\, t}{\partial\, ln\, x}\right)_F\, d\, ln\, x\right]$$
(12)

In above equation, similarity variable ξ is explicitly known. Thus, if self-similarity occurs, a further test is required for the new similarity variable, i.e., we have to see a plot of $F(x,t)$ versus ξ at different times showing a single collapsed curve. By using equation (12), equation (9) reduces to the modified population balance equation for breakage in self-similar form as,

$$\xi\, \varphi'(\xi) = \beta \int_0^1 \frac{\xi^2}{u^3}\, \varphi'\left(\frac{\xi}{u}\right)\, g(u)\, du$$
(13)

where u represents ratio of the breakage rate of the daughter particle to that of parent particle.

Inverse problem
For given self-similar curve in the form of φ versus ξ , we have to find constant β and function $g(u)$ over the unit interval [0,1].

III. Similarity Test

According to Narsimhan et al. [7, 6] and Brown and Glatz [2], if by translation parallel to the $ln\, t$ axis for the $ln\, t$ versus $ln\, x$ curves for different values of F, collapses into a single curve, it is said that self-similarity is there. In this translation, we have to choose a reference curve in which all other curves are translated and a reference particle size for the translation. However, there is a difficulty regarding reference particle size as most of the curves do not reach up to this size so that there is negligible overlap between the different curves due to which there is problem regarding translation distance. To overcome this difficulty, we take arc length for different $ln\, t$ versus $ln\, x$ curves. If similarity exits, the values of s(v), arc length, for different $ln\, t$ versus $ln\, x$ curves are the same at all $v = ln\, x$ values. For the curve $y = y(v)$, the arc length is given by

$$s(v) = \int_{v_0}^{v} \left[1 + \left(\frac{dy}{dv}\right)^2\right]^{1/2} dv$$
(14)

While calculating the arc length from experimental data, we face difficulty as the equation (14) contains derivatives of the curve. To avoid this difficulty, first of all, we fit a polynomial function for the different $ln\, t$ versus $ln\, x$ curves. It has been seen [3] that a quadratic curve is a best fit.

IV. Similarity Behavior Of Daughter Particle Distribution

A direct solution $\psi(z)$ of (1) for $b = 1/3,\ \gamma = 2$ [8] is

$$\psi(z) = 600\, z\, exp\left(-\, 60^{1/3} z^{1/3}\right)$$
(15)

From equations (2) and (15), we obtain:

$$f(x,t) = 600\, x\, (1 + 0.153261886478696\, t)^9\, exp\left[-60^{1/3} x^{1/3} (1 + 0.153261886478696\, t)\right]$$
(16)

For value of $f(x,t)$ in equation (16), we find the values of $b(x)$ and $w(x,x')$ in equation (1).

For this $f(x,t)$, cumulative volume fraction $F(x,t)$ is calculated as

$$F(x,t) = \int_0^x 600\, y^2 (1 + 0.153261886478696\, t)^9\, exp\left[-60^{1/3} y^{1/3} (1 + 0.153261886478696\, t)\right] dy \quad (17)$$

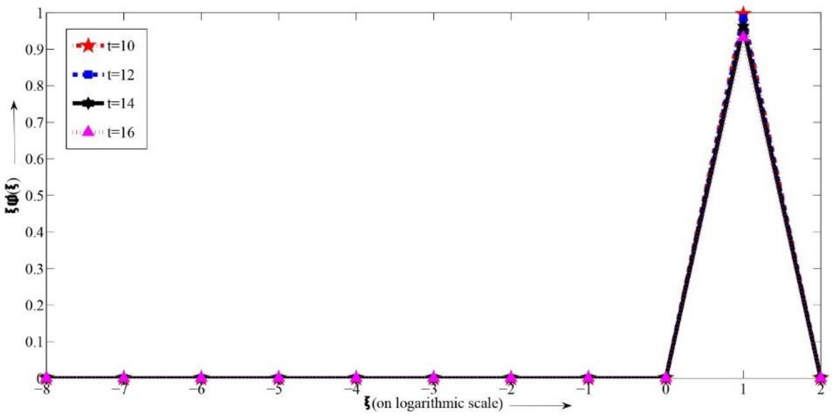
Now, using the transformation,

$$F(x,t) = \varphi(\xi),\ \ \xi = b(x)\,(1+t),$$

equation (6) reduces to the form of equation (13), where

$$\xi\, \varphi'(\xi) = 1800\, x^3 (1 + 0.153261886478696\, t)^9\, exp\left[-60^{1/3} x^{1/3} (1 + 0.153261886478696\, t)\right] \quad (18)$$

Now, we check for similarity of this transformation whether it is valid or not. For that we observe the graph of $\xi\, \varphi'(\xi)$ obtained using equation (18) given by:



This figure shows that the resulting distribution at four different times collapse into a single curve. So, it is a similarity distribution.

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