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Modeling of Granular Material Mixing Using Fractional Calculus

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Abstract – *Particulate and granular materials are found in different chemical processes. Measuring and characterizing the mixing degree remains a challenge, s it is an important variable for process performance. The availability of reliable sensors for real time control is still incipient or expensive, an alternative remains on the development of mathematical models for mixing prediction.The most commonly used approach for solid mixing concern on either diffusive or advective/convective processes. Fractional calculus represents a novel approach and a growing research field for process modeling, being based on derivates of arbitrary order. Therefore, it represents an important and alternative tool for mixing process modeling. This work study the use of a fractional diffusion model to describe granular mixing in a rotary cylinder, considering finite type of boundary conditions. Experimental data previously reported were used for validation purposes. The proposed approach could successfully describe the experimental data, thus, can be used as an alternative tool for mixing evaluation.*

Keywords*: Granular Material, Mixing, Fractional Calculus, Diffusion, Modeling*

Nomenclature

C	Tracer concentration	[$\mu g_{tracer}/g_{solid}$]
C_0	Initial tracer concentration	[$\mu g_{tracer}/g_{solid}$]
D	Diffusivity coefficient	[cm/s^2]
$E_{\alpha,\beta}(z)$	Mittag-Leffler function	
j	Counter	
t	Time	[min]
x	Axial distance	[cm]
z	Dummy variable	

Greek symbols

α	Fractional order of derivate
ϕ	Dummy variable
β	Dummy variable
Γ	Gamma function
π	Pi number

I. Introduction

Particulate and granular materials are frequently found in different chemical processes, going from polymer synthesis [1] to biotechnology [2]. However, one of the main difficulties is the measurement and characterization of mixing degree [3]. A poor mixture may lead, for example, low quality end-used properties of polymer based materials. It can also lead to lower reactant conversions due to a poor contact in case of chemical/biochemical reactors [4]. The availability of reliable sensors providing real-time information is an essential issue for process control [5]. Nevertheless, for solid mixing this type of sensor is still incipient or expensive [3], an alternative remains on the development of mathematical models for mixing prediction [6].

The most commonly used approach for solid mixing concern on either diffusive or advective/convective processes [7]. Usually, one of the components is considered a tracer and its concentration is evaluated throughout the mixing system by proper sampling devices and characterization [4]. Towards this, an "effective" diffusion coefficient is estimated aimed at an accurately description of the mixing behavior and a concentration profile. Literature reports several works on granular material mixing modeling by diffusion approach. More specifically, dealing with cylindrical geometry, Santomaso *et al.* [8],[9] report experimental results of solid mixing and further diffusive modeling validation, by using the classical diffusion equation and considering diffusion only axially. Recently, Marigo *et al.* [6] numerically studied the mixing behavior for granular mixing by using a Discrete Element Method.

Fractional calculus represents a novel approach and a growing research field for process modeling, being based on derivates of arbitrary order [10]. Literature reports different applications, for example in systems engineering [11], diffusion processes [12], heat transfer [13], among others [14].

Due to the heterogeneous nature of the granular material, memory effects can play an important role. Therefore, fractional calculus represents an important and alternative tool for mixing process modeling. Khan and Morris [15] reported the use of fractional differential equations for modeling solid mixing.However the boundary condition used in their work is not mentioned, but according to the reported results, it seems that the spatial variable was considered with infinite length, i.e., the boundary conditions were $C(t,x\rightarrow\pm\infty) = 0$, as the

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tracer particles were inserted in the center position, as shown by their results. On the other hand, it is important to note that finite type boundary conditions can be employed to describe a larger amount of physical systems, commonly used in chemical processes.

This work study the use of a fractional diffusion model to describe granular mixing in a rotary cylinder. Boundary conditions used considered spatial variable with finite length. Experimental data from Marsh *et al.* [4] were used for validation purposes. Consequently, this modeling approach can be used as an alternative tool for mixing evaluation.

II. Methodology

II.1. Experimental

Marsh *et al.* [4] studied the mixing o granular solid in a 80cm long, unbaffled drum rotated at 5 rpm the axial.According to the authors, wheat bran particles dyed with Rhodamine-WT were used as tracer. From distance 0 to 16cm of the axial length of the drum, only tracer particles were placed in, while from position 16cm up to the end of the axial length (80cm) normal particles filled the drum. Mixing degree was evaluated by characterizing sampleswithdrawn at positions 0cm; 16cm; 35cm; 50cm; 65cm. Further details regarding experimental procedure and characterization methods can be found elsewhere [1].

II.2. Modeling

As mentioned, a typical approach for modeling granular mixing concerns the hypothesis of diffusion phenomenon [7]. In order to generalized previously reported results [2]-[4], the proposed model for solid mixing is given by a fractional diffusion equation (1), which considers only axial diffusion, being radial mixing considered perfec.:

$$\frac{\partial^{\alpha} C}{\partial t^{\alpha}} = D \cdot \frac{\partial^2 C}{\partial x^2} \qquad 0 < \alpha < 1 \tag{1}$$

For modeling purposes, the following initial condition is given by (2), stating that only the initial portion of the drum has tracer particles:

$$C(t=0,x) = \begin{cases} C_0 & 0 < x < 16 \\ 0 & 16 < x < 80 \end{cases} \tag{2}$$

Boundary conditions are given by (3). Firstly, it can be seen that, differently from previously reported results [15], in this work, spatial variable was considered finite, ranging from x=0 to x=80. The boundary conditions used were also considered in different works [4],[8]-[9], resembling closed boundaries:

$$\left.\frac{\partial C}{\partial x}\right|_{x=0} = 0 \qquad \left.\frac{\partial C}{\partial x}\right|_{x=80} = 0 \tag{3}$$

The solution of the fractional differential equation (1) associated to the conditions given by (2) and (3) can be analytically obtained, yielding (4). More precisely, Separation variables method [16] can be used, the partial fractional differential equation splits into a fractional ordinary differential equation depending on time, which can be solve by Laplace Transform and a second order ordinary differential equation depending on the spatial variable, which, due to eigenvalues can be solved by Sturm-Liouville Problem [16]:

$$\begin{aligned} C(t,x) &= \\ &= C_0 \cdot \left[0.2 + \sum_{n=1}^{\infty} \left(\begin{array}{l} K_n \cdot \left(cos\left(\frac{n \cdot \pi \cdot x}{80} \right) \right) \cdot \\ \cdot E_{\alpha,1}\left(-\left(\frac{n \cdot \pi}{80} \right)^2 \cdot D \cdot t^{\alpha} \right) \end{array} \right) \right] \\ K_n &= \left(\frac{2}{n \cdot \pi} \right) \cdot sin\left(n \cdot \pi \cdot 0.2 \right) \end{aligned} \tag{4}$$

where:

$$\text{Mittag-Leffler function: } E_{\phi,\beta}(z) = \sum_{j=0}^{\infty} \frac{z^j}{\Gamma(\phi \cdot j + \beta)}$$

One can observe that if α=1, (4) results in the classical diffusion solution for the given initial and boundary conditions. Before performing parameter estimation, experimental data were normalized by dividing by the initial concentration, C_0, in order to avoid numerical convergence problems.

Parameter estimation tasks used minimum least squares as objective function and algorithms already used for fractional identification [11].

III. Results & Discussions

For the classical diffusion model α=1, Marsh *et al.* [4] estimated D = 9.15 cm^2/s. In this work, by proper parameter estimation, both α and D was infered and better prediction results were achieved byα=0.95 andD = 11.7 cm^2/s. It must be emphasized that the estimated D presents an overall feature as all experimental data were used for parameter estimation. A final value of 0.48 was obtained for the objective function.

Figs. 1, 2, 3, 4 and 5 present the simulation results and experimental data for the sampling points, for times up to 180 minutes after starting the cylinder rotation.

From these figures, it can be observed that model predictions agree with experimental data behavior.An equilibrium condition may be reached lead to a uniform C(t,x)/Co equal to 0.2, which truly represents the physical system, as initially 20% of the drum was filled with tracer particles (from position 0cm to 16cm), that will become mixed throughout the drum axial length. A value of 0.95 was obtained for parameter α.

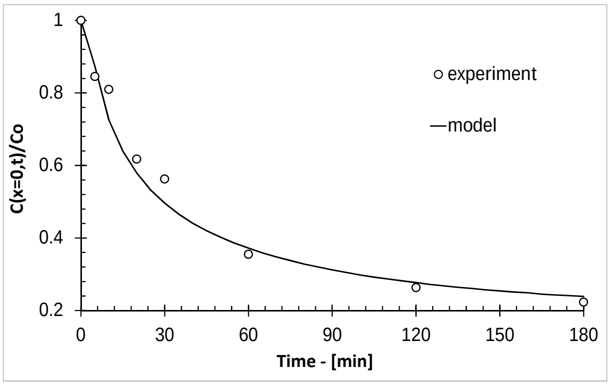

Fig. 1. Tracer concentration behavior for sampling position x =0cm

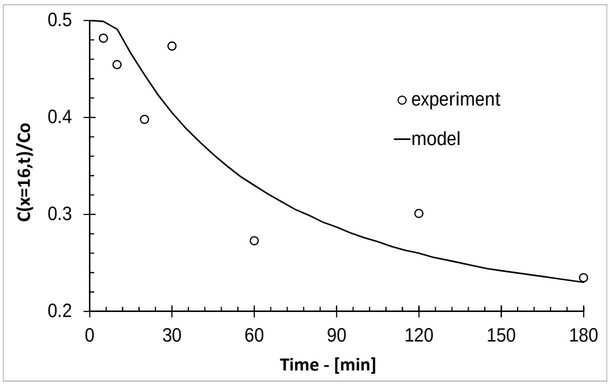

Fig. 2. Tracer concentration behavior for sampling position x = 16cm

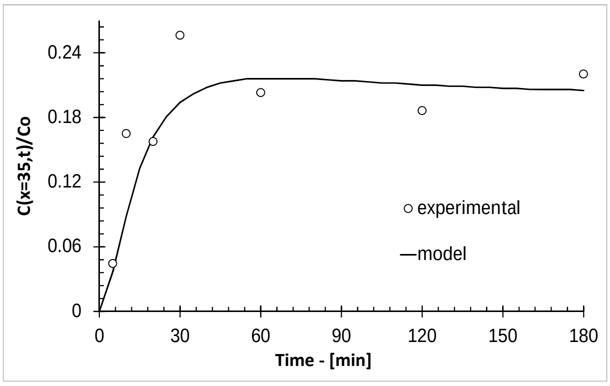

Fig. 3. Tracer concentration behavior for sampling position x = 35cm

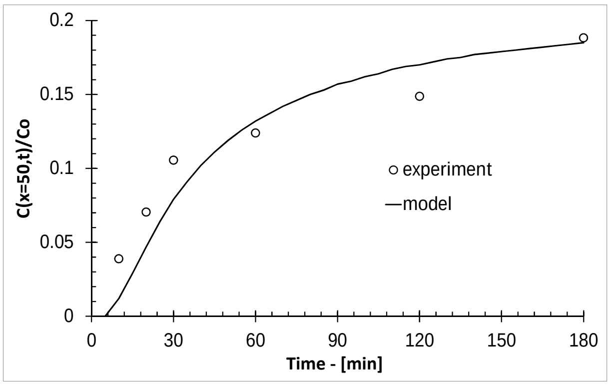

Fig. 4. Tracer concentration behavior for sampling position x =50cm

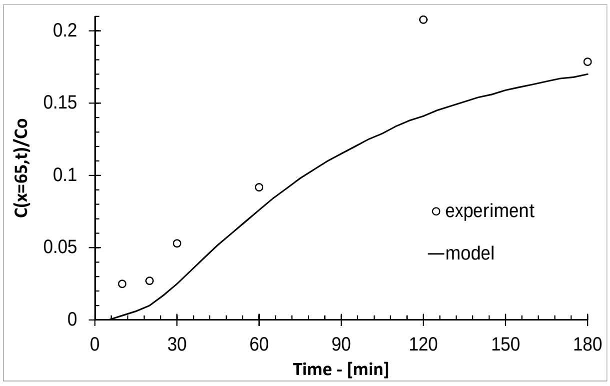

Fig. 5. Tracer concentration behavior for sampling position x = 60cm

Although close to 1, this estimated value shows that the mixing process may not follow a classical Fickian diffusion behavior, as reported by other authors [15]. This may happen, for example, due to heterogeneous nature of the solids used in the process. Finally, it is worth mentioning that memory effects may play a key role in the mixing process, leading to a fractional order for the diffusion equation.

IV. Conclusion

A new approach, based on fractional calculus, was use for solid mixing evaluation. Simulationswere performed in order to compare the proposed approach to experimental data. It was shown that the proposed fractional diffusion equation successfully describes the experimental data behavior, being an alternative tool for solid mixing evaluation.

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