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A measure of mixing from Lagrangian tracking and its application to granular and fluid flow systems

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ABSTRACT

This work concerns the development of two new indices that are extensive enough to be used to assess the mixing efficiency of both granular and fluid flow systems. They are based on the theory of principal component analysis and the concept of mixing in the weak and strong sense, and can be obtained from tracer trajectories (Lagrangian tracking) either numerically through computer simulation or experimentally by means of nonintrusive methods. It is explained how these measures, which in a way bridge the gap between global mixing properties and the local viewpoint of dynamical systems and chaotic theory, can provide the main mixing directions in a flow system and upper bounds for the mixing curves and mixing times. Two solid mixing cases and one fluid mixing case are presented to illustrate the wealth of detail provided by these two measures.

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1. Introduction

The development of measures to quantify mixing efficiency in granular and fluid flow systems has aroused interest for many years. Commonly used methods to assess the state of a mixture are based on sampling and the measurement over time of the concentration of a key component at various locations, in order to determine how fast the variance of the sample concentration values decreases to some expected value. Some of these methods are based on the use of probes, and the fact that they may alter the flow remains their main drawback. Optical techniques such as particle image velocimetry, are nonintrusive and provide relevant information about the flow dynamics. For the fluid systems, mixing times are generally obtained through techniques based on the addition of a liquid with a different property such as temperature (Lee and Yianneskis, 1997; Tanguy et al., 1992), pH (Cabaret et al., 2007; Delaplace et al., 2004) fluorescence (Houcine et al., 1996; Tanguy et al., 1998) or conductivity (Skelland and Moeti, 1989; Yakamura and Takahashi, 1999). Some of these approaches are however of limited use in the case of opaque systems. In solids mixing, the opacity of the system prevents observation of the particles that are deeper than just a few millimeters. In

this case, sampling can be achieved by means of thief probes but this technique is known to alter the state of the bed of particles (Brone et al., 1998) and does not provide information regarding the dynamical properties of the flow.

The experimental limitations described above can be alleviated by resorting to numerical simulation, that is CFD for fluid mixing and DEM (Discrete Element Method) for solids mixing, which have both proven efficient in describing the flow and mixing mechanisms in various fluid (a good review can be found in the Handbook of Industrial Mixing (Paul et al., 2004)) and granular systems (e.g. Bertrand et al., 2005). Another possibility consists of employing nonintrusive experimental techniques that allow for Lagrangian tracking and thus provide the trajectories of particle tracers in a flow system. Examples are the methods using radioactive tracers such as the positron emission particle tracking (PEPT) and radioactive particle tracking (RPT) methods. A good review of those nonintrusive techniques for the investigation of multiphase flow dynamics can be found in Chaouki et al. (1997).

Among the most commonly used measures of mixing based on sampling over time, as discussed above, are the intensity of segregation of Danckwerts (1952) and its variants, CoV (Coefficient of Variation) in the case of fluid systems or

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RSD (Relative Standard Deviation) in the case of granular systems, all of which evaluate the variance of the concentration of a given species in a flow system. Other mixing criteria have also been proposed in the literature. For instance, Asmar et al. (2002) investigated the mixing of particles in a vibrated bed by calculating the mean of the z-coordinates of the centers of a given particle type divided by the mean z-coordinate of all particles. Other mixing measures for particulate systems can be found in Poux et al. (1991). A good review of mixing indices in the context of fluid systems can be found in Hiby (1981).

The following remarks should be considered when measuring the mixing of liquid or solid mixtures:

- Frame invariance: the measure of mixing should be frame invariant with respect to rotation, translation, scaling or symmetry mapping.
- Spatial connection: many mixing criteria are not connected to spatial coordinates. These indices then fail in providing information as regards the main and secondary directions along which mixing occurs.
- Property connection: many mixing criteria are based on the concentration of a given species, that is one single property. In a lot of situations, more than one property should be considered at once to assess in a rigorous manner the state of mixedness of a system (e.g. temperature, particle size, particle density, particle color).
- Sample size invariance: the computation of the index of segregation or its variants depends on the number of samples considered. In the case of a granular system, it should be kept in mind that the asymptotic behavior of such measures of mixing depends on the number of particles in the sample (e.g. Lemieux et al., 2008).

In addition to the literature on the characterization of mixing and the evaluation of mixing time by means of spatial statistics, a large body of work has focused on the investigation of mixing properties using the dynamical system viewpoint and chaos theory. The emphasis is put on the analysis of local flow structures and their ability to enhance mixing (e.g. Meier et al., 2007; Ottino, 1989). Some chaotic properties of the flow can be derived such as its dimension, its entropy and its sensitivity upon initial conditions. However, this approach generally lacks in providing global measures of mixing, mixing curves for instance, because it addresses different (much smaller) time and spatial scales.

The objective of this work is to introduce new measures of mixing, applicable to both granular and fluid flow systems, which aim at bridging the gap between the global mixing properties and the local viewpoint of chaotic theory. More precisely, two different indices are defined, which are based on particle or tracer trajectories obtained either numerically through simulation or experimentally by means of nonintrusive methods. First, the concept of mixing in the weak and the strong sense is explained. It is then shown how these definitions and the theory of principal component analysis lead to frame-invariant mixing indices that are both extensive and quite general in scope. In particular, it is explained how these indices can provide an upper bound for the mixing curves and mixing times. Finally, the measures are applied, as an illustration, to three cases: (a) monodisperse particles in 2D and 3D tumblers with trajectories obtained experimentally by means of radioactive particle tracking (RPT), (b) bidisperse particles in a cylindrical drum with trajectories obtained numerically through a DEM

(Discrete Element Method) simulation, and (c) viscous Newtonian fluid in a Kenics static mixer.

2. Mixing definitions

Two definitions of mixing are first introduced. They are based on the trajectories of tracers or particles and the concept of stochastic independence. Let us consider N particles or tracers and denote by $\mathbf{x}^t(i)$ the position of particle i at time t . This particle follows a trajectory $\{\mathbf{x}^t(i)\}_{t \geq 0}$ that can be obtained either experimentally by various techniques (e.g. PEPT or RPT) or numerically through computer simulation.

Definition 1. Consider a probability measure \mathcal{P} . The system is said to be mixed in the weak sense if

$$\mathcal{P}\{\mathbf{x}^t(i)|\mathbf{x}^0(i)\} = \mathcal{P}\{\mathbf{x}^t(i)\}, \quad (1)$$

for each particle $i = 1, 2, \dots, N$.

This definition states that to be mixed in the weak sense, the distribution of particles at time t has to be independent of the initial distribution. In other words, the two distributions must not be correlated. Although it is quite general, it is based solely on the particle spatial coordinates. In some systems, this definition of mixing is not satisfactory because it does not characterize completely the state of mixedness of the particles. It is the case, for instance, of a particulate system where it is possible for the particles to distribute themselves in separated regions according to their size, their density, their color or some other properties.

Such a phenomenon is called segregation and is common in various industrial applications involving particles with different properties (e.g. pharmaceutical). As an illustration, Fig. 1 shows an example of the segregation of two sets of particles with identical particle size distributions (PSD) but two different colors, which are mixed in a tumbler. As can be seen, this system, which is spatially unmixed initially, ends up in a state where the particles are well mixed with respect to color (owing to the identical PSDs), but completely segregated with respect to size. According to the previous definition, the system is mixed in the weak sense. It is then clear that this definition fails to capture the state of segregation in this polydisperse system. This fact justifies the need for a definition of mixing that is wider in scope.

Definition 2. Consider a probability measure \mathcal{P} and $\mathcal{U} = \{u_1, u_2, \dots, u_K\}$ a set of time-independent particle properties such that $u_k(i)$ is the k th property of particle i . A system is said mixed in the strong sense if

$$\mathcal{P}\{\mathbf{x}^t(i)|\mathbf{x}^0(i), u_1(i), u_2(i), \dots, u_K(i)\} = \mathcal{P}\{\mathbf{x}^t(i)\} \quad (2)$$

for each $i = 1, 2, \dots, N$.

It then follows that any system that is mixed in the strong sense is also mixed in the weak sense. If Definitions 1 and 2 are satisfied, it means that the distribution of particles at time t is independent of the initial distribution with respect to both space and properties.

In the example related to Fig. 1, the properties of interest are particle size (u_1) and color (u_2). It appears that the system is only mixed in the weak sense since there is a correlation between the size of the particles and their location, which

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