Short communication

An analysis of the entropy of mixing for granular materials

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A B S T R A C T

Many existing definitions of the entropy of mixing for granular materials involve a "total entropy" that is calculated from the "local entropies" of all cells in the domain of the mixture. The total entropy has been used as a measure of mixedness by many authors, but they have virtually never presented the values of the individual local entropies. For comparison purposes, we introduced a parallel definition of the entropy of mixing by considering an alternative "total entropy" that is based on the "per-species entropies" of all types of particles in the mixture. Using a simple mixing model in continuous variables, we showed that the contributions of the individual "local entropies" and the "per-species entropies" to their respective totals show different trends during a specific, idealised mixing process: while the total entropy constantly increases following either definition, only the local entropies show non-monotonic changes; on the other hand, only the per-species entropies reach the maximum possible value of the Shannon entropy at the steady state of mixing. We rationalised these differences by considering the changes in the probabilities associated with each individual entropic term, in the context of the properties of the Shannon entropy, and confirmed these ideas by studying the two-dimensional phase-space trajectories of the individual entropic terms for the mixing process considered.

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1. Introduction: definition and some properties of the Shannon entropy

Since the concept of information entropy was put forward by Shannon in 1948 [1], many authors [2–10] have defined measures of mixedness based on the Shannon entropy for use in their study of granular mixing. We will first state the mathematical definition of the Shannon entropy. Consider a discrete probability distribution with n outcomes, with respective probabilities of occurrence given by $p_1, ..., p_n$; knowing exactly one of the n events is bound to occur, we define the Shannon entropy [1] of the distribution as

$$H = -\sum_{k=1}^{n} p_k \ln p_k \qquad (1)$$

Some important properties of the Shannon entropy [1] follow from this definition. Firstly, any change towards equalisation of $p_1, p_2, ..., p_n$ increases H, that is, if $p_1 < p_2$ and we increase p_1 and decrease p_2 by an equal amount so that p_1 and p_2 are more nearly equal, then the entropy increases. Secondly, when all the probabilities are made exactly equal, H reaches its maximum possible value of $\ln n$. Thus, H will keep increasing and ultimately reach its global maximum if and only if its associated probabilities constantly tend towards equalisation.

2. The "local entropy" concept

Consider a mixture of n_s different types of equal size particles, or "species". The entire domain that the particles occupy is divided into n_c fixed regions called "cells". Then most entropy-based mixing indices in the literature [2–10] are defined in a fashion similar to what follows: for a certain state of the mixture, one first calculates the "local entropy" for every individual cell using

$$S_i = -\sum_{j=1}^{n_s} p_{j/i} \ln p_{j/i} \qquad (2)$$

where i is the counter for cells, j the counter for species, and $p_{j/i}$ the conditional probability that a random particle picked from the mixture is of species j, given that the particle is in cell i; in order words, $p_{j/i}$ is the fraction of particles in cell i that are of species j. Next, one finds the "total entropy" of the entire mixture, given by

$$S_{\text{tot}} = \sum_{i=1}^{n_c} p_i S_i \qquad (3)$$

where p_i is the probability that a random particle picked from the entire mixture is from cell i, that is, the size of cell i divided by the size of the domain. We can think of S_{tot} as a weighted arithmetic mean of all S_i, where the contribution of each S_i is proportional to the size of cell i.

Although authors who proposed definitions similar to the above have closely examined S_{tot} during mixing, very little about the

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Table 1
Initial conditions of the mixing process considered in terms of $p_{j/i}$.

$p_{j/i}$		Cells		
		$i = 1$ (cell 1)	$i = 2$ (cell 2)	$i = 3$ (cell 3)
Species	$j = 1$ (blue particles)	1/18	0	11/18
	$j = 2$ (red particles)	0	1/18	5/18
	$j = 3$ (green particles)	17/18	17/18	1/9

individual S_i terms has been reported. We will now consider a specific example to examine the individual contributions of S_i to S_{tot}. Consider a mixture of different types of particles that are only

distinguishable by their colour: blue, red, or green, for which j is equal to 1, 2, or 3 respectively. Let p_j be the probability that a random particle picked from the entire mixture is of species j, and arbitrarily set $p_{j=1} = 2/9$, $p_{j=2} = 1/9$, and $p_{j=3} = 2/3$ for the purpose of illustrating the calculations. We divide the mixture into three equal size cells so that $p_i = 1/3$ for $i = 1, 2, 3$. Now consider a mixing process where the initial conditions are given by Table 1 in terms of $p_{j/i}$. Note it is possible to set p_j, p_i, and the initial values of $p_{j/i}$ to any other self-consistent values.

We now require a simple method to cause mixing of the particles. There are many methods of simulating granular mixing; some are very sophisticated, such as the Discrete Element Method approach
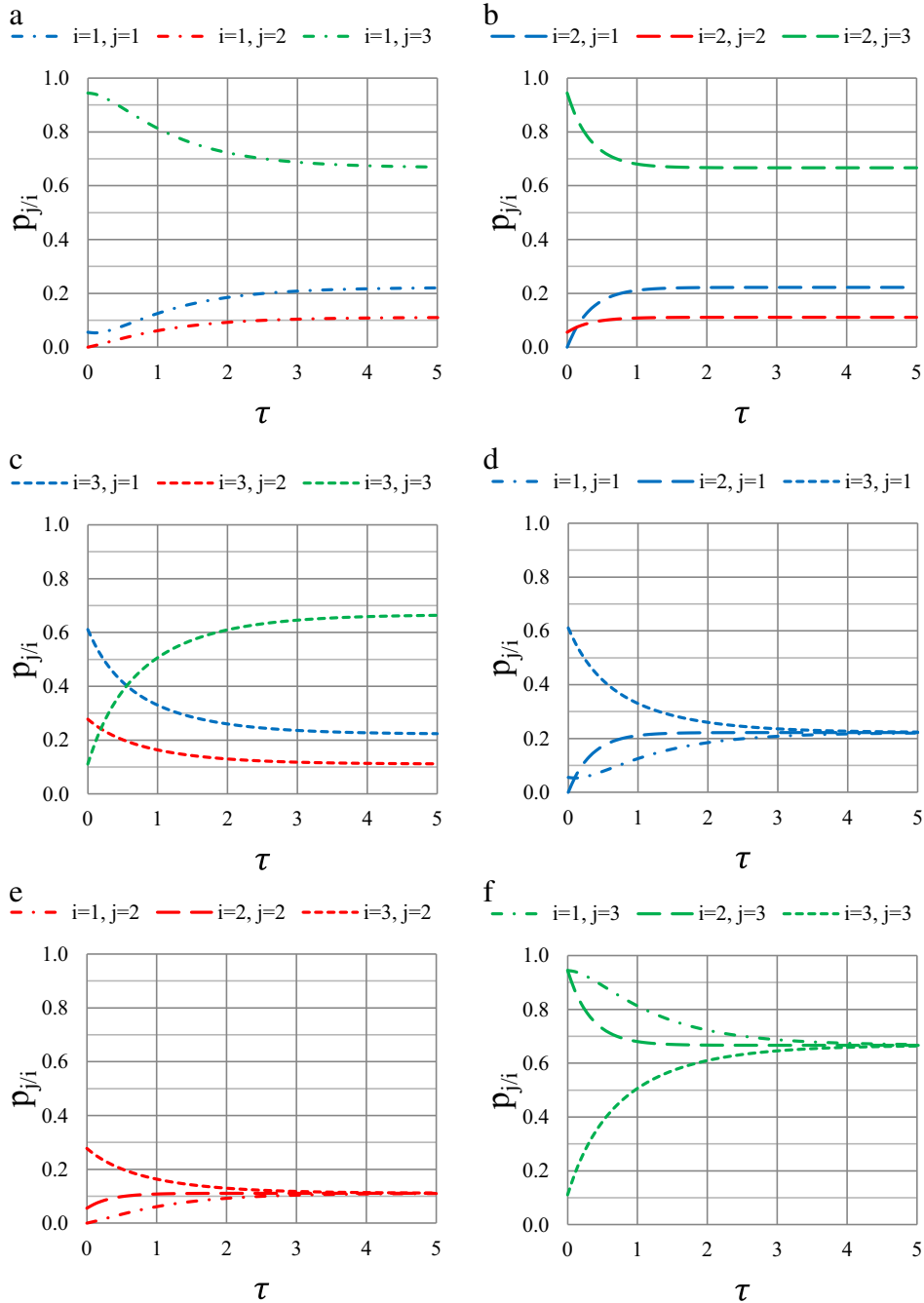
Fig. 1. (a). Solutions for the simulated mixing process in terms of $p_{j/i}$; cell 1, $i = 1$. (b). Solutions for the simulated mixing process in terms of $p_{j/i}$; cell 2, $i = 2$. (c). Solutions for the simulated mixing process in terms of $p_{j/i}$; cell 3, $i = 3$. (d). Solutions for the simulated mixing process in terms of $p_{j/i}$; blue particles, $j = 1$. (e). Solutions for the simulated mixing process in terms of $p_{j/i}$; red particles, $j = 2$. (f). Solutions for the simulated mixing process in terms of $p_{j/i}$; green particles, $j = 3$.