COMPLEX SYSTEMS

Researchers are investigating segregation and mixing phenomena in granular materials using a blend of theory, computations, and experiments. The foundations rest on a framework that has already yielded considerable insights into mixing of fluids and found applications in the fields as diverse as microfluidics, reaction engineering, polymer blending, and large-scale environmental processes.

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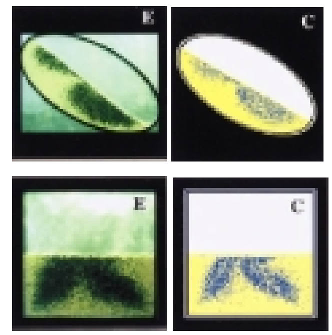
Objective: A system is termed complex when it consists of a large number of elements, called building blocks or agents, capable of exchanging stimuli with one another and with the environment. Complex systems display organization in the absence of any external organizing force, and their overall behavior cannot be described simply in terms of their building blocks; hence they must be analyzed as a whole. An example of a complex system is granular materials, which are ubiquitous in nature (*e.g.,* Earth sciences) and industry (*e.g.,* chemical, pharmaceutical, and advanced materials). The knowledge-base of granular materials, however, is disproportionately small and their fundamental understanding is very limited, which makes them an attractive research area for Dr. Ottino and his collaborators.



Experimental ("E") and computational ("C") results for half-full quasi 2-D tumbling mixers demonstrate competition between mixing and segregation.

Approach: The analysis relies on a combination of theory, computations and experiments. Computations involve the range of possible models: continuum descriptions, agent-based models and particle dynamics calculations. Granular material segregation experiments are conducted using a variety of non-cohesive beads in 2D, long-cylinder and full 3D containers. Images for quantitative analysis – degree of mixing and determination of various aspects of pattern structure – are compared with the results of simulations.

Results: Studies carried out by Dr. Ottino and his collaborators have revealed the complex interactions between chaotic mixing and segregation of several granular systems. Small differences in either the size or density of the particles have been shown to cause flow-induced segregation. Similar to fluids, non-cohesive granular materials can display chaotic advection; when this happens chaos and segregation compete with each other, giving rise to a wealth of experimental outcomes. Segregated structures, obtained experimentally, display organization in the presence of disorder that are captured by a continuum flow model, which incorporates collisional diffusion and density-driven segregation. These granular mixtures may be the simplest experimental example of a system that displays a competition between chaos and order. Remarkably the same nonlinear dynamic tools that are used to describe the chaotic flow of granular materials can also be applied to fluids, as evidenced by the successful modeling of chemical reactors and recent advances in microfluidic applications (*e.g., ex vivo* production of hematopietic cells in a series of parallel groves perfused by fluid flowing in the transverse direction).

Left: An initially well-mixed system of large and small particles segregates into a dynamic pinwheel structure upon tumbling.

Right: Visualization of a mixing structure in a 3D flow. The picture represents a slide through the flow obtained via a laser sheet. The image reveals islands of regularly and chaotic structures.

Selected Publications: Fountain GO, Khakhar DV, Ottino JM *Science* **1998**, 281:683; Hill KM, Khakhar DV, Gilchrist JF, McCarthy JJ, Ottino JM *PNAS* **1999**, 96(21):11701; Ottino JM, Khakhar DV *Ann. Rev. Fluid Mech.* **2000**, 32:55; Khakhar DV, Orpe AV, Ottino JM *Adv. Complex Sys.* **2001**, 4:407; Ottino JM and Khakhar DV, CHAOS **2002**, 12(2):400.