Journal of Thermodynamics & Catalysis

Pack, J Thermodynam Cat 2012, 3:3
DOI: 10.4172/2157-7544.1000e107

Editorial Open Access

Vital Molecules

George Pack*

Department of Chemistry, University of Louisville, USA

How is it that simple particles like atoms and small molecules move randomly yet molecules that are more complex can move in coherent patterns? Wanting to get a group of students to think about this, I went to early published work on Brownian motion. Robert Brown's 1827 paper [1] was titled "A Brief Account of Microscopic Observations on the Particles Contained in the Pollen of Plants; and on the General Existence of Active Molecules in Organic and Inorganic Bodies". Brown observed pollen grains and "other particles, at least as numerous, of much smaller size, apparently spherical, and in rapid oscillatory motion" in water and became convinced that the motion "belonged to the particle itself." Vitalism, which held that organic matter was fundamentally different from inorganic matter, influenced Brown. In this view, the emergence of complex order from elementary "organic molecules" in embryogenesis is similar to crystal growth from elementary "inorganic molecules". He wrote that, initially, "I was disposed to believe that the minute spherical particles or Molecules . . . were in reality the supposed constituent or elementary Molecules of organic bodies". With admirable diligence, Brown looked for active molecules and found that "on examining various animal and vegetable tissues, whether living or dead, they were always found to exist". He then found that inorganic matter, "rocks of all ages, including those in which organic remains have never been found, yielded the molecules in abundance . . . a fragment of the Sphinx being one of the specimens examined." Brown even showed experimentally that a single "active molecule" in a water droplet within an emulsion of water and almond oil moved "with undiminished activity", and so "attractions and repulsions among the particles themselves" did not drive their random motion. Pollen grains and other Brownian particles are not self-propelled. Eighty-two years after Brown's paper, Einstein and Smoluchowski explained the origins of Brownian motion as interactions with solvent molecules.

Having moved beyond vitalism, we now accept a common set of elements for inorganic and organic matter. There remains, of course, a distinction between nonliving and the living matter. Contrast stochastic chemical diffusion with the emergence of self-organized collective coherent motion (flocking) of birds, fish, insects, bacteria and other creatures. The former belongs in chemistry and physics while the latter has long been the province of the life sciences. But, as recent studies with self-propelled molecules (protein motors) have been showing, the two phenomena have much in common. The flocking of creatures can clarify the origins of collective motion of molecules.

Models that successfully explain flocking have been around since the late 1980s when Reynolds [2] introduced a computer-simulation of "boids". The algorithm had three rules: avoid collisions with nearby flockmates; match velocity with nearby flockmates; and, stay close to nearby flockmates. Long-range coherence arises through these short-range interactions. In 1997, Vicsek [3] proposed a two-dimensional non-equilibrium model in which self-propelled particles move on a plane with a constant velocity and locally interact with their neighbors by moving in the direction equal to the average direction of their neighbors. Making the connection to classical physics, the authors noted that the model is analogous to a Monte Carlo realization of a classical ferromagnet in which the individual magnetic spins develop long-rang order through nearest neighbor interactions. In 2007, Cucker and Smale [4] extended this model to three dimensions and added a scaling of interactions that depended on the square of the interparticle distances. These models have been remarkably successful in capturing the essence of flocking behavior.

Still, there is a gulf between geese and molecules. Surprisingly, the key to organized coherent motion is not intelligence - bacteria also flock. For our purposes the main difference is that geese are self-propelled while simple molecules are passive, getting their motion from stochastic bombardment by other particles. The model of "Active Brownian Particles" of Romanczuk *et al.*[5] is a concept based on models more physical than mathematical. An active particle is subject to stochastic thermal fluctuations as well as having "an internal energy depot and/or a (nonlinear) velocity-dependent friction function". The key to this model is that the particles are subject to active fluctuations that "point parallel or perpendicular to the time-dependent orientation of the particle" [6]. There is a nonrandom component to the movement of active particles.

Active molecules are self-propelled - is this enough to enable flocking? Biological molecular motors are proteins that convert chemical energy to motion. The energy source is typically the hydrolysis of adenosine triphosphate, ATP. The complexity of living cells makes it impossible to isolate the coherent motion of just these motors but several ingenious experiments have taken these systems out of their cellular environment. Several motor proteins move along the cytoskeleton, scaffolding made of protein filaments. Myosin, powered by ATP, glides along the thinnest to these filaments, the linear actin protein polymer. Essentially reversing the roles of the players, two groups [7,8] in 2010 immobilized myosin on coverslips and added actin filaments. The filaments, driven by the myosin motors, spontaneously formed two-dimensional coherently moving structures that changed over time. More recently, Sumino *et al.* [9] immobilized the ATP-powered molecular motor dynein, which "walks" along the thickest cytoskeletal filaments, microtubules. Adding microtubules to the immobilized dynein resulted in microtubule-dynein binding but there was no motion without APT. On addition of the ATP fuel, the microtubules self-organized into vortexes that evolved over time with individual microtubules circulating "inside one vortex for some time

***Corresponding author:** George Pack, Department of Chemistry, University of Louisville, USA, Tel: +(502) 852-6798; Fax:+ (502) 852-8149, E-mail: george.pack@louisville.edu

Received May 03, 2012; **Accepted** May 08, 2012; **Published** May 08, 2012

Citation: Pack G (2012) Vital Molecules. J Thermodynam Cat 3:e107. doi:10.4172/2157-7544.1000e107

before moving to a neighboring one or travelling farther and starting to revolve around some more distant core." This molecular motion rivals that of flocks of birds in its coherence (although perhaps not in its purposefulness).

The distinction between active self-propelled molecules and simple passive ones updates the vitalists' distinction between "organic" and "inorganic" molecules. Passive molecules undergo Brownian motion, but active, self-propelled molecules (molecular motors) can self-organize like flocks of birds. The puzzle of the emergence of coherent collective motion of active particles may yet be analogous to emergence of the static crystalline order of passive molecules from the liquid phase.

References

1. Brown R (1827) from The miscellaneous botanical works of Robert Brown: Volume 1 (John J. Bennett, Ed.) R. Hardwicke, London (1866).
2. Reynolds CJ (1987) Computer Graphics. 21: 25-34.
3. Czirok A, Stanley HE, Vicsek T (1997) Spontaneously ordered motion of self-propelled particles J Phys A- Math and Gen 30: 1375-1385.
4. Cucker F, Smale S (2007) Emergent Behavior in Flocks. *IEEE Trans, Automat Control* 52: 852–862.
5. Romanczuk P, Bar M, Ebeling W, Lindner (2012) Active Brownian Particles. From Individual to Collective Stochastic Dynamics. Eur Phys J Special Topics 202: 1-162.
6. Romanczuk P, Schumansky-Grier L (2011) Brownian motion with active fluctuations. Phys Rev Lett 106: 230601.
7. Butt T, Mufti A, Rosenthal PB, Khan S, Khan S and Molloy JE (2010) Myosin motors drive long range alignment of actin filaments. J Biol Chem 285: 4964-4974.
8. Schaller V, Weber C, Semmrich C, Frey E, Bausch AR (2010) Polar patterns of driven filaments. Nature 467: 73-77.
9. Sumino Y, Nagai KH, Shitaka Y, Tanaka D, Yoshikawa K, et al. (2012) Large-scale vortex lattice emerging from collectively moving microtubules. Nature 483: 448-452.