Researchers Find Order, Beauty In Chaotic Chemical Systems

Chaos research yields insights into complex chemical phenomena that previously were inaccessible to scientific scrutiny.

Stu Borman, C&EN Washington

One might expect research on chaos to be a frustrating, fruitless field of study, perhaps even an unscientific one. But when researchers in nonlinear chemical dynamics look at chaotic chemical systems, they see much more than just the confusion and unpredictability that might be expected. Instead, beneath a thin veneer of chaos, they see surprising order, richly detailed structure, and striking beauty.

"I really feel like we're on a new frontier of science," says chemistry professor Kenneth C. Showalter of West Virginia University in Morgantown. "It's how the people in the '20s must have felt when they were working out the details of quantum mechanics. Nonlinear dynamics in chemistry, physics, and biology really is a science revolution. It seems like everything we look at is new—not just in the sense of refining something we already knew, but astonishing."

"Chaos, in the scientific sense of that term, isn't easy to define. A chaotic system is one that acts irregularly and exhibits extreme sensitivity to initial conditions, but whose behavior is actually deterministic—that is, describable by mathematical equations, often very simple ones."

"A chaotic system looks to be completely random," explains Richard J. Field, a chemistry professor at the University of Montana, Missoula, "but in fact it's deterministic because it represents a solution to a set of differential equations. In such a set of equations, you plug in the initial conditions and the equations will tell you how the system is going to evolve from that point on."

However, the problem with chaotic systems, he says, "is they're very, very sensitive to initial conditions; you can't know the initial conditions carefully enough to actually predict what's going to happen. Two very close together solutions will diverge. That divergence is measured by something called a Lyapunov exponent. If it's positive, then they will diverge, and the bigger it gets the faster they'll diverge."

The discovery in the 1960s of deterministic chaos forced a major change in the philosophy of science. Until then, it was an article of faith that the future behavior of any nonquantum mechanical system could be predicted, assuming equations describing its evolution could be derived and a complete description of its current state (initial conditions) was available. However, a chaotic system is unpredictable unless its initial conditions are known with infinite accuracy—an impossible task. Thus, chaos theory, like the Heisenberg uncertainty principle in quantum mechanics, sets limits on what is knowable.

"Deterministic differential equations, says Showalter, "have been the cornerstone of our predictive ability in physical science ever since Newton's time. But now we know that chaotic solutions are nonpredictable, that there is an inherent uncertainty in nature that comes out of deterministic chaos."

For example, because of sensitive dependence on initial conditions, weather can be predicted with accuracy for only a few days. Physicist Harry L. Swinney of the University of Texas, Austin, estimates that a computer with as many transistors as there are atoms in the universe would be able to make accurate weather predictions only about 14 days in advance.

In chemistry, chaos appears in systems that oscillate in concentration, potential, or some other parameter. For example, chaos can manifest itself as a state of irregular, unpredictable oscillations in a reaction undergoing periodic changes in the concentration of intermediates. Chaos has been seen in reactions on surfaces, such as in the electrochemical dissolution of metals. Chaos has also been found in the vibrational quantum states of molecules.

The oscillations of a chaotic system may at first follow almost the same trajectory as that of a nonchaotic system. However, predicting the trajectory of a chaotic system in the long term, says chemistry professor John Ross of Stanford University, "gets more and more difficult, more and more expensive. You need higher and higher precision because two neighboring trajectories will diverge exponentially."

Although "chaos" has become a convenient catchphrase, researchers in the field are quick to point out that it is a misnomer. "It's an unfortunate label," says Showalter, "because chaos is usually associated with complete disorder."

In fact, deterministic chaos involves motion that is orderly. This is in contrast to noise, which stems from random forces. "If you think of a phase space of chemical concentrations," says Ross, "noise will fill that space, meaning sooner or later you'll go to every point in that space. That's not true with chemical chaos. Chaotic systems are attracted to a surface of fractal dimension. They're well ordered."