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Research News

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CHAOS THEORY IN CHEMISTRY:

RESEARCHERS MUST FIND NEW WAYS

TO DESCRIBE CERTAIN CHEMICAL REACTIONS

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Chemists may have to find new ways of describing certain non-linear chemical reactions, thanks to the new science of chaos.

Advanced and developed over the past 20 years, chaos is the study of non-linear phenomena that share such common characteristics as randomness and extreme sensitivity to fluctuations so small that they would be ignored by classical physics. Scientists have discovered chaotic behavior in a number of natural systems, including weather patterns, heart rhythms and animal populations.

Chemists at the spring meeting of the American Chemical Society will be told that chaos may also exist in certain chemical reactions -- though it is not easy to find. Chaotic chemical reactions will require new methods for measurement and description, though some existing experimental tools may still be useful.

"There are aspects of non-linear chemical reactions that may be made intelligible by using the kinds of study techniques chaos researchers use," said Dr. Ronald F. Fox, a physicist and chaos researcher at the Georgia Institute of Technology. "It's been taken for granted that the way to describe these reactions is known, but that's just not true any more."

Fox believes chaos may be found in the continuous chemical reactions which take place in flow-though tanks. If any of the reactants are added periodically, Fox said, the reaction could become chaotic. Because the outcome of such reactions cannot be predicted, he suggests chemical manufacturers using such reactions should take steps to prevent chaotic chemical activity.

Fortunately, scientists can anticipate which reactions might be susceptible to chaos by studying the normal fluctuations in the chemical system. Fox has found that the intrinsic molecular fluctuations indicated by the chemical equation are mathematically related to the Lyapunov exponent, the technical "litmus test" for the presence of chaos.

Most chemical reactions can be described with relatively straightforward equations. A quantity of one material reacts in a predictable way with a quantity of a second material to produce a predictable quantity of a third material. At the end of the reaction, the material assumes an equilibrium state at which no further reactions take place.

On the surface that may be true, but on a microscopic scale, things can be dramatically different, Fox said.

Even at apparent equilibrium, sensitive light-scattering instruments still detect significant molecular activity. Though such activity is of no importance in most cases, those tiny perturbations can quickly be magnified into large and significant fluctuations if the system becomes chaotic.

In a linear process, two chemical reactions that start out nearly similar produce nearly similar outcomes. But in chaotic system, small initial differences quickly become dramatic differences in ways that are not predictable. This "divergence of trajectories," characteristic of chaos, is expressed as the Lyapunov exponent.

"When you have a chaotic system, the fluctuations that are normally very small become very large," Fox explained. "There is extreme sensitivity to the initial conditions, and that sensitivity shows itself in the growth of the fluctuations."

When the fluctuations in a chemical system become large, the "mass-action" equations normally used to describe them lose their validity. While Fox has not yet determined how these chaotic systems can be characterized, he believes the focus will have to shift to the microscopic level where the fluctuations began.

What will chaos mean to chemists?

"You don't see chaos in your ordinary reactions," Fox explained. "Chemists don't have to junk their laboratories if they do this sort of thing, but they can't analyze their data quite so straightforwardly."

Analytical tools based on light scattering or neutron scattering can be used to observe chaotic behavior because they measure the microscopic molecular activity that is magnified in chaos, Fox said. The amount of light scattering is directly related to the level of chaotic activity, and can therefore provide a quantitative measure of it, he explained.

Fox takes exception to much of the "chaos" study underway in colleges and universities, suggesting that "what many researchers are calling chaos is not chaos at all." He questions scientists who claim an ability to predict future activity through an understanding of chaos.

"One of the principal lessons about chaos is that it is unpredictable," he said. "This high sensitivity to initial conditions makes the outcome very unpredictable."

Fox will be part of a "Pedagogical Symposium" with seven other scientists discussing aspects of chaos. The symposium will take place April 23 at the ACS Spring Meeting in Boston.