Researchers bridge the gap between disciplines to better understand chemical reactions

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Simon Fraser University researchers are yielding new insights into how chemical reactions can be understood and guided. Results of their

interdisciplinary approach have been published in *Physical Review Letters.*

Though chemical reactions may be very complex, they often follow a series of elementary steps as they progress. In their work, SFU chemistry Ph.D. student Miranda Louwerse and physics professor David Sivak found that information provided by a reaction coordinate about how a reaction is progressing precisely equals how dissipating that coordinate is.

Their findings indicate a deep connection between two previously distinct fields of physics—stochastic thermodynamics, which describes energy and information changes, and transition-path theory, which details reaction mechanisms.

Discovering a link between these two fields has allowed the pair to create a framework to quantify the information about a reaction contained in system dynamics, which provides a physical understanding of what it means for particular dynamics to be relevant for that reaction.

This understanding is particularly useful in helping researchers navigate massive datasets.

The researchers note that advances in computing are making it easier than ever to simulate complex systems and chemical reactions, but along with useful information these simulations can produce huge amounts of extraneous data. This framework can help researchers separate signal from noise, enabling them to track exactly how a reaction unfolds.

In the future, this will help researchers and engineers better identify bottlenecks in the production of chemicals, making it easier to design interventions that will allow more control over reactions.

Through guided design, they will be able to achieve faster and cheaper production of chemicals with less waste. It can also guide a more thorough understanding of how pharmaceutical drugs work in the body, suggesting pathways toward developing drugs with less harmful side-effects.

This insight also raises some intriguing possibilities for more communication between and among disciplines. Establishing the fundamental equivalence between basic concepts in distinct fields helps theorists apply established theory from one field to the other. This opens up opportunities to adapt methods for measuring energy dissipation to identify reaction mechanisms, and may yield further insight in the future.

"We weren't looking for this," Sivak says. "We found it in the course of studying something else. But it fits well in our broad research area understanding the interplay of energy, information, and dynamics in biological function at the molecular level."

More information: Miranda D. Louwerse et al, Information Thermodynamics of the Transition-Path Ensemble, *Physical Review Letters* (2022). DOI: 10.1103/PhysRevLett.128.170602

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