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New molecular modeling techniques for catalysis in unmixed systems

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Scientists at the U.S. Department of Energy's Ames Laboratory have developed molecular modeling simulations and new theoretical formulations to help understand and optimize catalytic reactions that take place in chemical environments where the reactant "ingredients" for catalysis are not well mixed.

In catalysis a chemical reaction is accelerated by adding another component, the catalyst, which remains unchanged during the reaction. In many cases, such as when the catalytic reaction takes place in a solution, the reactants are able to mix together easily (and are sometimes stirred to ensure mixing). This mixing is assumed in standard theories of chemical kinetics that describe how quickly and efficiently catalytic reactions occur.

But not all catalytic reactions occur where ingredients are able to mix. For instance, catalytic reactions to create fuels in mesoporous particles and to remove pollutants in high-pressure surface reactions happen in unmixed systems. And for those cases, the standard analysis of chemical kinetics needed to be refined.

In papers that appeared recently in *Chemical Reviews* and the *Journal of Chemical Physics*, Ames Laboratory chemists Jim Evans, Dajiang Liu and their research team focused on modeling reactions in three classes of catalytic environments where chemical components do not easily mix. For two classes, catalysis in narrow pores of mesoporous particles and catalysis on metallic surfaces exposed to high pressure, crowding prevents reactants (and products) from moving enough to mix. The third class is surfaces under low pressure, where interactions between the adsorbed reactants themselves cause these species to organize into ordered domains or "islands" rather to than mix randomly.

"For all of these scenarios, there are many 'extra' steps in the overall catalysis reaction process that must be built into chemical simulation models to reliably describe these systems that are not well stirred," said Evans. "For example, for catalysis within crowded narrow pores, we simulate the entrance of the reactant into the pores, diffusion within the pore, conversion of the reactants to products within the pore, and diffusion out of the pore, rather than just assuming 'well mixed' conditions. All of these steps control the catalytic yield for these unique reaction processes. All of them must be built into the simulation models."

The result is comprehensive molecular-level simulations that more accurately and realistically describe what is going on in non-stirred catalytic systems.

"The simulations can play the role of 'numerical experiments,' meaning if we do our work right, rather than having to do an experiment in a lab, our models can tell us what these types of catalytic reactions will do."

Evans' team also refined existing analytic theories of catalytic reaction rates so that they can be better applied to unmixed systems.

Provided by Ames Laboratory

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