Popular Science Summary

Steering ammonia oxidation: how temperature picks the products on a palladium catalyst

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Catalysts are silent helpers in modern life. They sit inside the exhaust pipe of every car, turning toxic gases into harmless ones, and they sit inside huge industrial reactors, turning the nitrogen in air into the ammonia that goes into fertilizer. Without catalysts, modern food production and clean air would not be possible.

This thesis looks at one specific step in fertilizer production: the oxidation of ammonia (a compound of nitrogen and hydrogen) on a hot metal catalyst into nitric oxide, which is later converted into nitric acid, the starting material for nitrogen fertilizer. The catalyst used in industry is usually platinum; we worked with its sister metal palladium, which follows closely related chemistry. When ammonia meets oxygen on a hot palladium surface, three different things can happen. The ammonia can turn into nitric oxide (NO), which is what industry wants because it leads to fertilizer. Or it can turn into nitrogen gas (N_2), which goes back into the air without doing much. Or it can turn into nitrous oxide (N_2O), a strong greenhouse gas that we want to avoid.

Which of these three products comes out of the reaction depends on how hot the palladium is and what the surface looks like at that moment. To make more of the useful product and less of the harmful one, we need to know exactly what is happening on the catalyst as the reaction runs.

To watch the reaction in real time, we used a special technique at the MAX IV synchrotron in Lund, Sweden. The synchrotron produces very bright X-rays that let us see which atoms are sitting on the surface of the palladium and which gases are floating just above it. We squirted short bursts of ammonia onto the catalyst hundreds of times in a row and accumulated snapshots across all the bursts, gaining enough signal to build a movie of how the surface and the gas change together, with about ten frames per second.

At 500 °C, the palladium surface is mostly oxidized, almost like rust, and the reaction produces a mix of all three nitrogen products. At 600 °C, the surface is mostly metallic, and almost everything that comes out is the useful nitric oxide. Two surprising things happen between the two temperatures. First, less ammonia reacts at the higher temperature, even though one might expect a hotter surface to be more active. The reason appears to be that the oxygen atoms sitting on the cooler, oxidized surface help break ammonia apart, and this assistance is lost once the surface turns metallic. Second, even though less ammonia reacts at 600 °C, the same fraction of the supplied oxygen is consumed at both temperatures. Making nitric oxide costs more oxygen per ammonia molecule than making the other two products, so the shift toward nitric oxide compensates for the drop in ammonia conversion. The two effects pull in opposite directions and, by coincidence, nearly cancel each other out.

Understanding why a catalyst makes one product over another, and how this changes when the gas supply is not steady, is one step toward designing cleaner and more efficient industrial reactions.