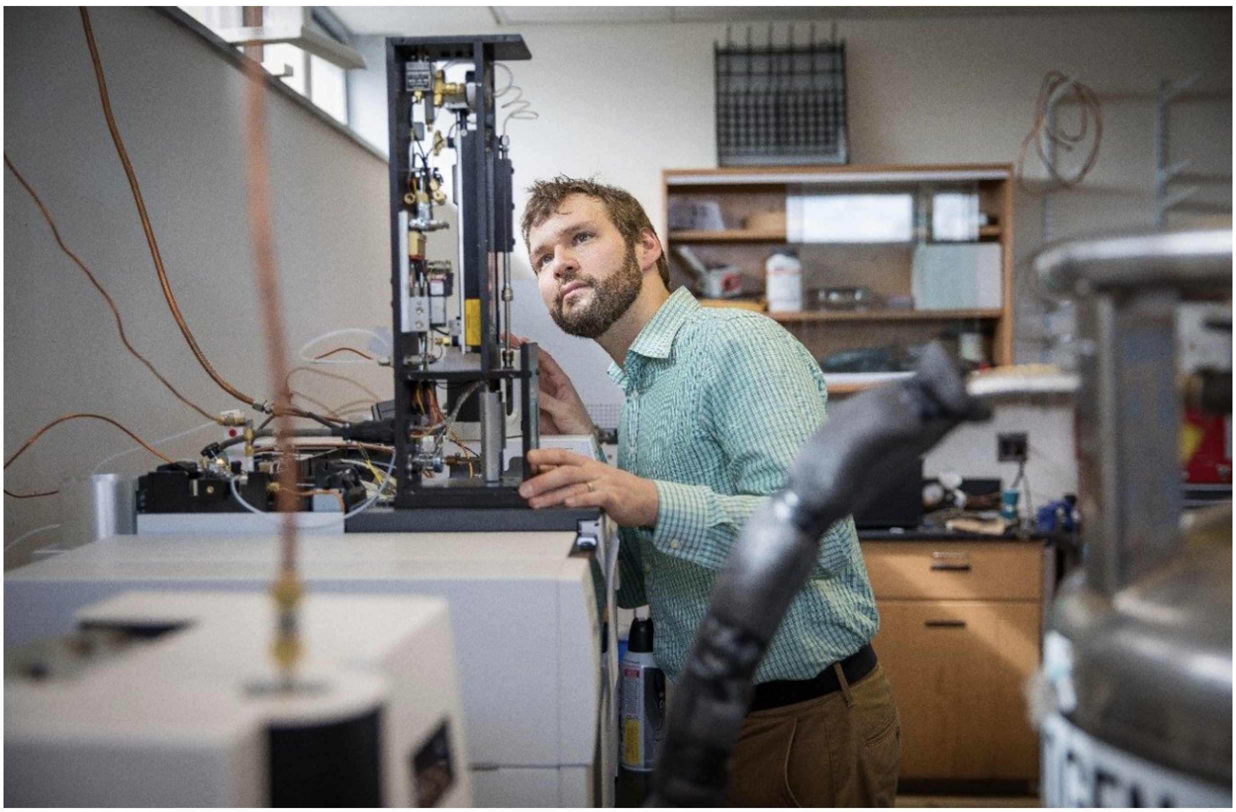
Method of tracking reactions between air and carbon-based compounds established

February 26 2018



Gabriel Isaacman-VanWertz arrived at Virginia Tech a little over a year ago, but the new assistant professor brought with him research that may alter the way researchers study air. Credit: Virginia Tech

By being the first to fully track the changing chemistry of carbon molecules in the air, a Virginia Tech professor could change the way we study pollutants, smog, and emissions to the atmosphere.

Gabriel Isaacman-VanWertz, lead scientist on a new study published in *Nature Chemistry* and assistant professor in Virginia Tech's department of civil and environmental engineering, has established a method of tracking reactions between air and carbon-based compounds—a feat that has been previously elusive to researchers.

This new finding could allow researchers to study pollution, smog, and haze in a comprehensive way, backed by data that accurately depicts a compound's behavior over time.

"There are tens of thousands of different compounds in the atmosphere," Isaacman-VanWertz said. "In general, the focus of my work is to study the chemistry of how those tens of thousands of compounds interact with each other and change with time."

When a certain compound is introduced into the atmosphere, it chemically reacts to form other compounds and molecules over time, explains Isaacman-VanWertz, who began this research as a post-doctoral research fellow at the Massachusetts Institute of Technology with study co-author Jesse Kroll.

Isaacman-VanWertz is particularly focused on studying the way the atmosphere interacts with organic compounds—the carbon-containing compounds that make up all living things. Large amounts of these compounds are emitted from natural sources and human activities.

Anything with a scent emits organic compounds: citrus, vinegar, nail polish remover, and gasoline, for example. Once these emitted compounds enter the atmosphere, they change in complex ways to form hundreds or thousands of other compounds.

Previously, tracking the way the carbon changes once it enters the atmosphere has been a challenge. Thanks to tools developed in the past decade, this study found that complete measurement of carbon in the atmosphere is now possible, though it still requires state-of-the-art instruments and careful analysis.

For this project, Isaacman-VanWertz studied the smell of pine, which is made of an organic compound known as pinene.

Isaacman-VanWertz and his collaborators at MIT used five spectrometers—advanced pieces of equipment that classify chemicals by their masses and the atoms they contain—to measure the characteristics of carbon inside a Teflon bag the height of a person in a climate-controlled, blacklight-outfitted room.

When they turned on the blacklights, it was like turning on the sun, Isaacman-VanWertz said. The light of the "sun" spurred the chemistry of the pinene inside the chamber and simulated the reactions that would occur in the atmosphere.

Each spectrometer was tasked with collecting a certain set of data throughout the elapsed reaction, like tracking specific ranges of chemical compounds. One of the hardest parts of this experiment was putting all of these measurements on the same scale, Isaacman-VanWertz said. Understanding the specific details and measurements of each instrument can be so complex, he said, there are doctoral students writing entire theses on these topics.

Isaacman-VanWertz and his collaborators were able to, for the first time, fully track the carbon in the pinene molecules from start to finish as they underwent chemical changes as they would in the atmosphere. The carbon atoms in pinene do not disappear after their initial introduction to the atmosphere—they turn into hundreds of different compounds through a cascade of chemical reactions.

Although the initial mixture of compounds formed from reactions of pinene is very complex, all the carbon was found to end up in "reservoirs" that are relatively stable and won't react further in the atmosphere.

What's more, the process is likely similar for other carbon-based compounds. Isaacman-VanWertz picked pinene because it has been extensively studied, so he could use previous work to make sense of his observations.

Though pinene is naturally emitted, its behavior is comparable enough to better anticipate the way other compounds, like those in pollutants, smog, and haze, will react in the air. Understanding this helps "paint a big picture of the atmosphere," Isaacman-VanWertz said.

For example, these results will help other researchers understand how pollutants from a power plant might transform in the atmosphere and impact a downwind community.

"If you can understand how the chemistry happens, then you can understand what sorts of pollutants will be in the atmosphere based on how far from a polluting source you are," Isaacman-VanWertz explained.

Isaacman-VanWertz hopes other researchers will build upon the results of this study. He wants to know whether the tendency of emitted compounds to end up as long-lived atmospheric components is generally applicable to other compounds and how this process might coexist or compete with other processes occurring in the atmosphere.

More information: Gabriel Isaacman-VanWertz et al, Chemical

evolution of atmospheric organic carbon over multiple generations of oxidation, *Nature Chemistry* (2018). DOI: 10.1038/s41557-018-0002-2

Provided by Virginia Tech