Simulation reveals molecular footprint of organic air pollutants

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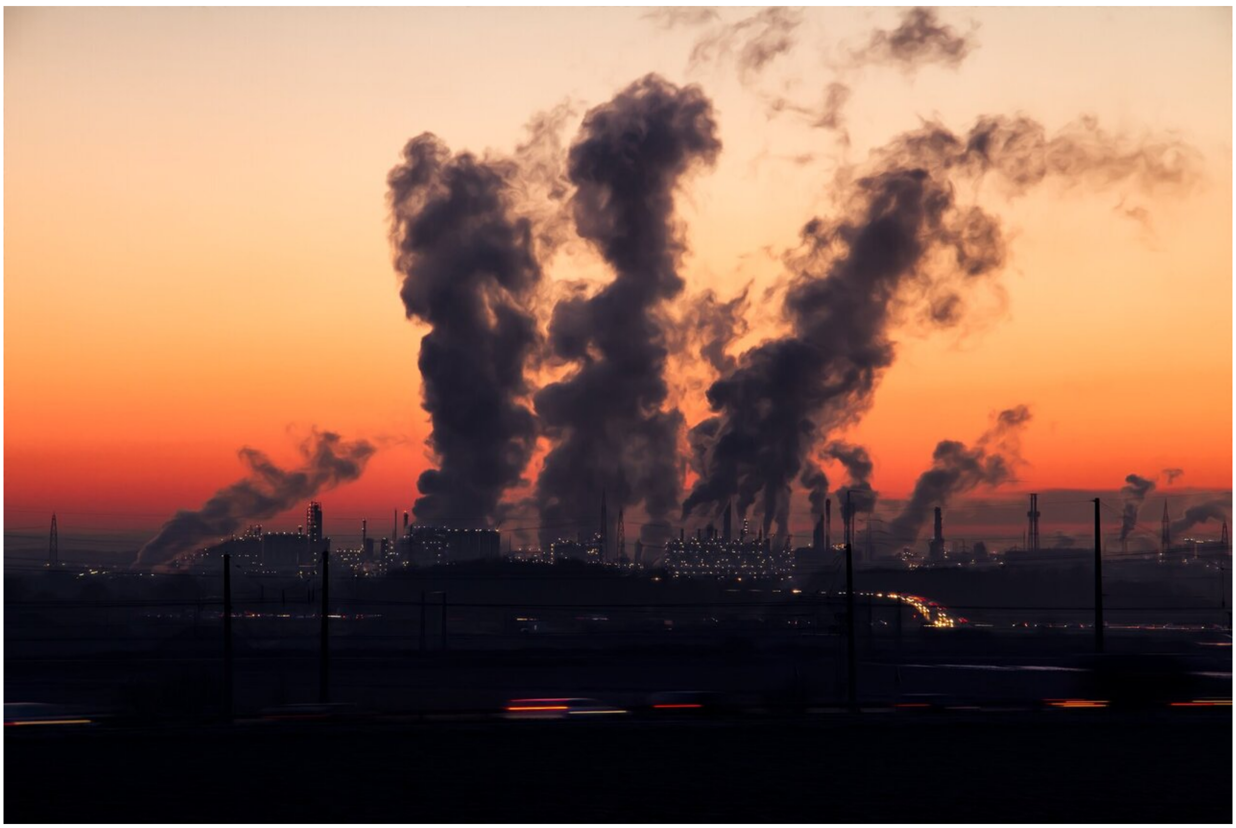

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Joining the global effort to curb air pollution, researchers at Texas A&M University have developed computational tools to accurately assess the footprint of certain organic atmospheric pollutants. Their simulation, described in the journal *Environmental Science and Technology*, could help government agencies keep a closer check on human-made sources of carbon-based pollutants.

"Human activity has led to a substantial increase in organic air pollutants, like aerosols, which has caused a deterioration of air quality in many places around the world and even changes in climate," said Dr. Qi Ying, associate professor from the Zachry Department of Civil and Environmental Engineering. "But by gaining a better estimate of organic aerosols through specific marker compounds, we can develop better emission control measures for cleaner air for all."

According to published reports, 20-40% of the particulate matter in the lower atmosphere comes from organic aerosols. Air pollution contributed by these compounds is an ongoing menace that affects climate, health and visibility. For example, depending on the type of aerosol, some can change the amount of heat coming into the atmosphere, while others influence the quantity of heat leaving. Also, organic aerosols can be inhaled easily and, if present in the body in high enough concentrations, can worsen many health problems from asthma to chronic obstructive pulmonary disease. These compounds can also reduce visibility by causing haze.

Organic aerosols begin their journey into the atmosphere as volatile compounds that are released into the air from a variety of natural and human-made sources, such as burning fossil fuels and vehicle emissions. These precursor aerosols then react with oxidants and condense onto existing particles in the atmosphere to form secondary organic aerosols. Thus, from an air quality management's perspective, Ying said it is necessary to know which precursors contribute to the build-up of secondary organic aerosols so that their specific sources can be curtailed.

The extent of certain precursor aerosols is calculated from the ratio of the abundance of a marker molecule called 2,3-dihydroxy-4-oxopentanoic acid (DHOPA) to the amount of secondary organic aerosol in air samples from field experiments. Historically, this ratio is determined using laboratory test chambers wherein very controlled atmospheric conditions are maintained. However, the ratio may not be suitable for use in different atmospheric conditions in the field.

"We really don't know whether this ratio is fixed or changes in the open environment," said Ying. "In ambient air humidity, temperature and other climatic factors change continuously which, in turn, could impact the estimates of the concentration of the secondary organic aerosols."

To overcome this drawback, the researchers used a supercomputer at the High Performance Research Computing facility at Texas A&M to simulate the atmospheric chemistry based on the ambient conditions over East Asia, including China, Japan and Korea. As inputs, the simulation was given information on where the emissions are coming from, the emission rates and the meteorological data at different locations. The simulation focused on how much secondary organic aerosols are formed from different precursors, particularly the ones that contained the molecular signature, DHOPA.

Upon running the simulations, the research team found that the ratio varied with the ambient temperature and the levels of organic aerosols in the air. They also observed that the ratio determined from previous chamber studies would lead to significant errors in the estimation of secondary organic aerosols without a correction. However, for regions with comparable levels of air pollution, the correction for the ratio remained the same.

"We have come a long way in reducing inorganic air pollutants, but as the contribution of these compounds becomes smaller, a much higher fraction of air pollution will be from organic precursors," said Ying. "We have started with DHOPA as a marker for some precursor aerosols but would like to identify molecular markers for other precursors, which still remains to be done."

More information: Jie Zhang et al, Estimation of Aromatic Secondary Organic Aerosol Using a Molecular Tracer—A Chemical Transport Model Assessment, *Environmental Science & Technology* (2021). DOI: 10.1021/acs.est.1c03670

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