Air quality tests need simplifying to help reduce dangerous emissions

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New methods of testing and simulating air quality should be considered in order to help policy makers have a more accurate understanding of how emissions affect air pollution levels, new research suggests.

In a review published in the *Journal of the Air & Waste Management Association*, the authors claim that current air quality modelling systems used in the US to perform simulations to help us understand how pollutants react in the atmosphere need to strike a balance between sufficient chemical detail and needless speculation to produce accurate results to help improve air quality.

The new paper provides recommendations for how to produce more accurate descriptions of atmospheric chemical reactions, and in-turn air quality simulations, in the fight to reduce dangerous emissions.

The production of air pollution from motor vehicles, industrial power plants, and fossil fuel emissions are determined by complex chemical reactions. To accurately simulate air pollution, air quality models solve sets of equations that mathematically describe the physical and chemical processes regulating the fate of emissions in the atmosphere. Lead author Professor William Stockwell from the University of Texas at El Paso explains, accurate simulations of air pollutants require updated and accurate descriptions of the chemical processes for the changing chemical regimes of the atmosphere and emerging contaminants of concern.

Researchers compared current techniques used to describe atmospheric chemical reactions against more historical techniques. They focused their comparison on techniques used in a three-dimensional model commonly used by environmental agencies to simulate ozone, particulate matter, and atmospheric acid concentrations, and develop effective emission reduction strategies.

According to the review, early development (1970-2000) of techniques for describing atmospheric chemical reactions involved adding a chemical reaction one-by-one to the mathematical description, each followed by laboratory testing using an environmental chamber, and comparing the simulations with the results. "We consider this to be a "bottom-up" approach," says Stockwell.

In comparison, the current techniques for describing atmospheric reactions are referred to as a "top-down" approach and involve first creating highly complex mathematical descriptions of chemical reactions prior to testing and then later simplifying them for their use in an air quality model.

The researchers were both surprised and concerned to find that the top-down approach has been widely advocated to the exclusion of the "bottom-up" approach" for updating the descriptions of the chemistry used for air quality modeling.

Stockwell argues that starting the development of the mathematical description of the chemistry with a very large number of reactions that are not well tested in the laboratory, may add an unnecessary amount of uncertainty to the description of the chemistry in the model that, in turn, may impact a model's effectiveness at simulating air pollution.

Instead, the researchers suggest that air quality models would be more accurate if the descriptions of atmospheric chemical reactions were developed through a combination of bottom-up and top-down techniques, i.e., adding a reaction or small group of reactions to the mathematical description (bottom-up technique), followed by testing against more complex mathematical descriptions (top-down) and a final simplification for air quality model input.

The researchers also recommend that more attention should be given to alternative techniques to produce the sets of equations that mathematically describe the chemical processes for air quality modeling, such as the use of informatics and air quality modeling systems that better characterize the uncertainty in their simulations.

More information: William R. Stockwell et al, A Perspective on the Development of Gas-phase Chemical Mechanisms for Eulerian Air

Quality Models, *Journal of the Air & Waste Management Association* (2019). DOI: 10.1080/10962247.2019.1694605

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