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Viewpoint

Assessing Air Quality Impacts of Greener Chemicals: Beyond Traditional Metrics

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Air quality has serious consequences for human health and well-being. It has recently been estimated that poor air quality is responsible for 7 million excess deaths per year,[1] with increasing links also being drawn between air quality and mental well-being.[2] Across the world, and particularly the global south, there is abundant evidence and recognition of poor air quality as an important risk factor for human health.[3−7] The photooxidation of volatile organic compounds (VOCs) is the primary source of hazardous substances such as secondary organic aerosol, tropospheric ozone, and particulate matter in populated areas. Successful regulation has significantly reduced VOC emissions from traditional sources such as transport and fossil fuel processing, yet emissions from solvents, agrochemicals, adhesives, and other VOC-emitting products remain persistent and increasingly dominate total non-methane VC emission.[8] These humanmade emissions are collectively termed volatile chemical products (VCPs) by the atmospheric chemistry community.[9−11] While attention is paid to the atmospheric implications of new chemical products at the level of industrial regulation, this generally takes the form of reactive measures. New products are usually checked against lists of restricted ozone-depleting or high-global warming potential (GWP) substances such as those listed in the Montreal protocol,[12] the Kyoto protocol,[13] and their various amendments. Beyond this, neither the U.S. Toxic Substances Control Act (TSCA) nor the EU regulation on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) mandate testing of the atmospheric photooxidation of new chemicals, despite requiring extensive testing of biodegradation and toxicity in other environmental domains.[14−17] Instead, non-methane VOCs are typically regulated at the point of emission based on their emitted mass, with little attention paid to their diversity in structure and reactivity.[18,19] VCPs in particular contain a significant fraction of heteroatom-containing and multifunctional compounds, and thus, one cannot assume that their reactivity is the same as that of classical, hydrocarbon-dominated VOC sources. There is therefore a need for a more proactive evaluation of the potential tropospheric air quality impact of new chemicals during early design protocols to help mitigate potential harm postcommercialization.

Green chemistry is central to the transition away from the unsustainable practices of the present, having led the way in developing renewably sourced, energy efficient, safer, and more biodegradable chemicals and processes. There is, however, a concerning lack of consideration of the atmospheric fate of newly developed chemicals during most early design processes. Toxicity and mutagenicity are regularly considered alongside the sustainability of new chemicals. While it has been common for many groups to use biodegradability (measured, modeled, or assumed) as a sole measure of environmental fate, we now believe that this approach is inadequate. Jessop and MacDonald have proposed a hotspot-driven framework[20,21] in which research priorities are identified by considering the interaction between the multiple stages that define a product life cycle. Within this framework, it stands to reason that if a chemical's primary fate is release to the atmosphere as a VCP (as is the case for many volatile and/or nonpolar compounds such as solvents), then its atmospheric reactivity is likely to be a direct hotspot. By contrast, focusing on the biodegradation of such compounds in irrelevant environmental domains such as water or soil has limited merit. This blind spot may stem in large part from the lack of collaboration between two seemingly aligned fields. A vast majority of those working in atmospheric chemistry have backgrounds in physical, theoretical, and/or analytical chemistry, and while green chemistry is diverse in those it attracts, in our experience it remains dominated by those with training in materials, organic chemistry, and catalysis. We have observed that the lack of network overlap between these two groups can at times be a

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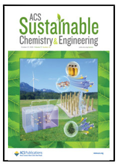

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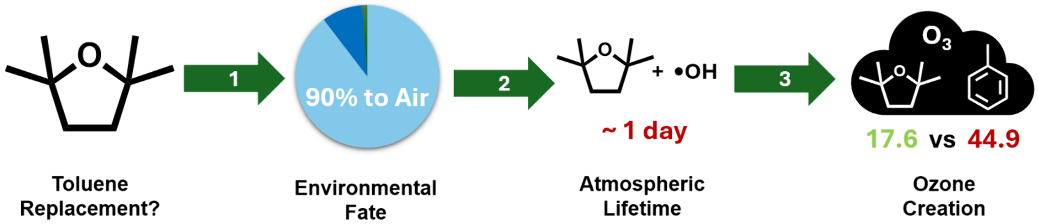

Figure 1. Our workflow to screen for problematic air quality impacts in new chemicals, illustrated with the biobased solvent TMO (2,2,5,5-tetramethyloxolane). SARs suggest that TMO, while volatile and reactive, is still significantly less ozone-generating than the toluene it is intended to replace.

significant barrier to initiating collaboration, which we believe is crucial to addressing the complex and multidimensional problems found in sustainability research.[22]

For several years, we have been working to bridge this gap, focusing on investigating the atmospheric breakdown of various biobased solvents during their design and development, yielding a range of interesting and unexpected kinetic data, mechanistic insights, and atmospheric implications.[23−25] In our work to date, we have often found that biobased solvents are similarly or less harmful than the solvents they are intended to replace, but this is not always the case. The unorthodox molecular structure of some substances can give rise to unexpected photooxidation pathways with dramatic negative effects on air quality. The atmospheric photooxidation of agrochemical VCPs has also received significant attention in recent years,[26−29] unveiling complex reactivity and secondary pollutant production stemming from the wide range of functional groups and heteroatoms typically incorporated into such compounds. Particularly problematic links can be drawn between the preference for photochemical stability in agrochemical design protocols[30−33] and the resulting tendency for the persistence of pesticides in the atmosphere allowing for their long-range transport and magnified negative impact on air quality, human health, and the environment.[34,35] Such findings strengthen the case for the inclusion of explicit atmospheric fate analysis into the early design processes of new chemicals, to avoid unforeseen environmental hotspots. Experimental studies on gas phase photooxidation are, however, complex and time-consuming and thus inaccessible to nonexperts, or those wishing to screen large numbers of compounds early in a design process. Fortunately, there are a plethora of accessible and freely available tools available to estimate parameters relevant to atmospheric chemistry.

So how can molecular design strategies avoid negative air quality impacts?

In our view, there are three key metrics that should be employed (outlined in Figure 1). Step-by-step guidance on the estimation and interpretation of these is provided in the Supporting Information. First, it is important to understand where a chemical ends up (i.e., air, water, soil, and/or sediment) when released to the environment. For this purpose, we find the fugacity model of Parnis and co-workers[36−38] suitable for a first pass, being both powerful and easy to use. Ideally, the inputs for this model would be measured experimentally; however, in the likely case that some of these data are not available, they can be readily estimated. For this, the combination of structure−activity relationships (SARs) available in the U.S. EPA EPI Web package[39] is free to access and provides good quality data from only a SMILES code or drawn structure.

The second key parameter is the gas phase rate coefficient for the reaction of a VCP with the hydroxyl radical (k_{OH}). Reaction with hydroxyl radicals is the dominant sink for most organics in the atmosphere as they are generated in high concentrations by sunlight-initiated reactions between oxidants such as O_3 and NO_2 and water. OH radicals are far more reactive with VOCs than their precursor oxidants. Accurately estimating k_{OH} allows the calculation of a range of atmospheric parameters, including the lifetime of a VOC in the troposphere. For estimating k_{OH}, we recommend the SAR developed by Jenkin et al.,[40,41] which can be accessed via the web-based implementation of the GECKO-A model[42] made available by Paris-Est Créteil University.[43] This tool also converts the rate constant into an atmospheric lifetime automatically for easy recognition of very long-lived species that have the potential to act as greenhouse gases.

The final metric we routinely use is the estimated photochemical ozone creation potential ($POCP_E$). This is a combined estimate of the amount and rate of ozone generated by a given VOC in the troposphere, which is an effective proxy for most other negative air quality impacts (e.g., aerosol, smog, etc.). This value can be straightforwardly obtained via a SAR from Jenkin et al.,[44] using the previously estimated rate constant and some basic structural information. This powerful descriptor can be used in isolation (as a rule of thumb we view a $POCP_E$ of 1−30 as good, a $POCP_E$ of 30−60 as poor, and a $POCP_E$ of >60 as highly problematic) or to directly compare a potential substitute to the compound it is intended to replace, with a lower value being preferred.

Further atmospheric metrics such as global warming potential (GWP) and ozone depletion potential (ODP) may be crucial in a minority of cases; however, the majority of (nonhalogenated) VOCs are nowhere near long-lived enough to act as potent greenhouse gases or deplete stratospheric ozone. Ensuring new chemicals have a lower $POCP_E$ than the compounds they are intended to replace is therefore of primary importance.

We strongly encourage the community to factor these three metrics (proportion lost to the atmosphere, atmospheric lifetime, and $POCP_E$) into their design processes and use them as quantitative metrics to assess the relative greenness of new compounds.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssuschemeng.5c08649.

Step-by-step guidance on estimating and interpreting three air quality metrics (proportion lost to the atmosphere, atmospheric lifetime, and $POCP_E$) (PDF)

Spreadsheet tool for POCP_E estimation (XLSX)

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Author Contributions

The manuscript was prepared by J.D.M., with contributions from all authors. Our work in this area was originally conceived by C.R.M. and T.J.D., with significant subsequent input from J.R.S.

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Notes

The authors declare no competing financial interest.

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