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## Indoor Air Quality through the Lens of Outdoor Atmospheric Chemistry

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### Abstract

Outdoor atmospheric chemistry and air quality have been the topic of research that intensified in earnest around the mid-20<sup>th</sup> century, while indoor air quality research has only been a key focus of chemical researchers over the last 30 years. Examining practices and approaches employed in the outdoor atmospheric chemistry research enterprise provides an additional viewpoint from which we can chart new paths to increase scientific understanding of indoor chemistry. This chapter explores our understanding of primary chemical sources, homogeneous and multiphase reactivity, gas-surface partitioning, and the coupling between the chemistry and dynamics of indoor air through the lens of outdoor atmospheric chemistry. The means to mitigate degraded air quality outdoors are heavily rooted in public policy actions, while the commercial sector mainly promulgates solutions for indoor air quality, making practical and actionable outcomes to research essential for prompt improvements to indoor environments. Indoor and outdoor environments have many important scientific distinctions, but a shared vision for healthy environments motivate both research communities in the same way.

### Introduction

Air quality has been of general public awareness for centuries, but only became clearly codified over approximately the last 150 years. In the late 19<sup>th</sup> century, actions to address public health during intense urbanization were based, at least in part, on the human sense of smell in the waning years of adherence to miasma theory (Kiechle 2017). The notion that exposure to ‘bad air’ was a risk for contracting disease was broadly replaced by germ theory. Modern understanding of infectious disease, indeed, includes the possibility that a subset of known infectious diseases can be spread through exposure to airborne biological particles. However, a general sense of healthfulness continues to be connected with our sense of smell as a detector of air quality, both indoors and outdoors. Important health effects of poor air quality are also associated with exposure to *chemical* agents, rather than just biological ones; poor air quality is associated with various non-communicable diseases and is a leading global health risk factor (Murray et al. 2020).

Scientific understanding of outdoor air quality has grown significantly since the mid-20<sup>th</sup> century. Tracking radiogenic isotopes released from atomic bomb detonations allowed for new insights on long range transport (Burton and Stewart 1960). Around the same period, smog formation represented an intense health and safety problem in major cities like Los Angeles and London; similar air quality problems persist to varying degrees to this day in urban environments around the globe. Arie Haagen-Smit’s discovery of the photochemical processes that created smog and recognition that ozone played a central role in urban air pollution (Haagen-Smit and Fox 1956) were critical achievements in establishing the importance of

chemistry in atmospheric phenomena that degraded air quality. Following growing scientific understanding, along with dedicated efforts to communicate these findings, government regulations and public policy have been used to address outdoor air quality problems to impressive effect (Hand et al. 2020). Key advancements in chemical analysis technology continue to allow for an ever-increasing level of detail in our understanding of atmospheric chemistry through increases in sensitivity, portability, spatial/temporal coverage, and chemical specificity to target measures that will help to mitigate poor air quality.

Building science and indoor air quality have also advanced dramatically since the mid-20<sup>th</sup> century. Specific studies of indoor chemistry began in the 1970's and have been accelerating especially since the mid-1990's (Weschler 2011). In the same period, however, improvements to building technology and energy efficiency have advanced more rapidly than methods to thoroughly understand and address indoor air quality from a chemical perspective. It remains critical to increase our understanding of indoor chemistry and clearly communicate new knowledge to the public. Significant progress has been made in elucidating the chemistry that occurs in both the gas phase and on surfaces indoors. More recent applications of highly sensitive, specific, and rapid on-line chemical measurements of the gas phase, aerosol particles, and surfaces have continued to enhance our depth of understanding (Farmer 2019). Since improvements in indoor air quality are promulgated by the building industry, researchers need to continue to develop a clear and predictive understanding of the processes that lead to degraded air quality along with solutions for practitioners to implement. Therefore, the outcomes and goals of indoor chemistry studies differ slightly from outdoor air, where changes in public policy are often a more crucial element of effective solutions.

In this chapter, we seek to unpack the approaches of outdoor atmospheric chemistry research with an eye toward their application to future studies of indoor air chemistry. The objective within each topical section is to explore several ways in which outdoor atmospheric chemistry has been conducted; examples have been chosen such that they shed light on the way that indoor chemistry is currently studied or could be studied in the future.

### **Primary Chemical Sources**

Introduction of outdoor air is an important chemical source for indoor air. At the same time, mounting evidence shows the growing importance of indoor activities and emissions of volatile chemical products on outdoor air quality (McDonald et al. 2018). Processes that add chemical constituents to the air are important controlling factors in atmospheric chemistry and often represent the most viable opportunity for mitigating poor air quality. Considering only primary (i.e. direct) emissions, sources are often categorized as 'natural' or 'anthropogenic,' although the line can be blurred in some cases, like agriculture, wildfires, or land-use change. Each source has its own chemical signature, including but not limited to: a wide variety of volatile and semi-volatile organic compounds (VOCs and SVOCs: hydrocarbons, carbonyl compounds, organic acids, amines) including compounds that are considered to be persistent organic pollutants; oxides and/or oxoacids of sulfur ( $\text{SO}_2$ ,  $\text{H}_2\text{SO}_4$ ), nitrogen ( $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{HNO}_2$ ,  $\text{HNO}_3$ , organic nitrates), or carbon ( $\text{CO}$ ,  $\text{CO}_2$ ); inorganic acids ( $\text{HCl}$ ,  $\text{H}_2\text{S}$ ,  $\text{HCN}$ ) and bases ( $\text{NH}_3$ ); and aerosol particles of organic, inorganic, biological, mineral, or mixed composition (Finlayson-Pitts and Pitts 2000). The source signatures of many types of anthropogenic sources can be replicated in laboratory settings if they are associated with engineered systems (e.g., combustion engines). However, deviations in emission strengths or chemical composition between controlled laboratory operating conditions and less-controlled field operation can be important (Frey et al. 2003; Gentner et al. 2017). Natural sources of aerosols and gases to the outdoor environment can be more challenging to simulate and study in a controlled manner. Emission processes can be the result of nuanced couplings between physical, chemical, and biological processes, along with a wide variety of spatial (nanometer to kilometer) and temporal (second to year) scales.

To account for couplings between ambient environmental conditions and emission source signatures, field experiments are targeted for strategic or opportunistic sampling of the atmosphere. Anthropogenic sources can be probed over timescales in which variations in activity are either predictable or known externally, such as weekday/weekend studies or episodic shutdowns/reductions of source activity, like the public response to the COVID-19 global pandemic (Kroll et al. 2020). Field experiments, in some cases, yield less specific chemical information than is achievable in laboratory studies due to various confounding environmental factors, but provide key constraints and guidance for more fundamental study and continued model development. Improvements in transportable and field-deployable chemical measurement technology have enabled major advances, allowing for online measurement approaches to field campaigns that were previously restricted to laboratory studies or offline operation (Laskin et al. 2018). Supplementing field observations with controlled laboratory experimentation using emission source simulators can yield a greater depth of fundamental understanding, but are often subject to a variety of their own caveats. However, coordinated combinations of field measurements, laboratory studies, and modeling have provided significant insight on complex atmospheric chemistry topics (Burkholder et al. 2017; Ault et al. 2020).

It is possible for indoor air quality to bridge the gap between field and laboratory studies more readily than outdoors, as perturbations to the indoor environment can be made deliberately. Two key approaches to perturbing indoor air composition are available: enhanced ventilation or air cleaning to rapidly reduce concentrations of compounds that are more abundant indoors than outdoors, and source modulation that can provide episodic additions of chemical constituents to indoor air. Each of these approaches can yield important insights about emission rates and rapid post-emission processes like chemical reactions or phase partitioning that act as sinks for aerosol particles or traces gases of interest. At the same time, care must be taken to understand the realism of the perturbation strength. Comparison of deliberate perturbations to indoor air composition and chemical processes should be compared against measurements of opportunistic perturbations due to non-prescribed occupant activity or normal building system operations. Modulation of HVAC operating status (cooling and heating cycles), window opening, day/night temperature and light cycles, and occupant cooking or cleaning activities are key opportunities for study.

The concept that source emission and physicochemical processes near to the chemical source can respond to the environment has been noted indoors in the context of relative humidity (RH) and temperature (T) for some gases (Parthasarathy et al. 2011) and aerosol particles (Xie et al. 2007; Salimifard et al. 2017). Emission source behavior studies in realistic environments are important to perform, despite being subject to complication by interfering chemical signals or poorly-constrained sink processes that influence airborne constituent concentrations. Complementary use of controlled source characterization studies in the laboratory environment using smaller or more controllable chambers allows for deeper inspection of fundamental principles, while implementation of similar experiments in more complex, realistic indoor environments allows for an accounting of rapid interactions between the source and/or freshly emitted material with the realistic surroundings, providing an ‘effective’ source strength.

Additional complexity beyond varying RH and T are possible. Studies of biosphere-atmosphere coupling in the outdoor environment require careful accounting for biogeochemical processes in terrestrial or marine environments. For instance, chamber studies of biogenic VOC production from plants may constrain emission rates, which can then be juxtaposed with emission estimates derived from ambient measurements of the same VOCs in or near a forest canopy outdoors. The field studies of ambient air may, for instance, make clear that measurements that account for stress responses, including those arising from herbivory or disease, are necessary (Faiola and Taipale 2020). In addition, meteorological conditions can influence the behavior of biological systems that drive emissions, and atmospheric conditions also influence the chemistry that may occur. For some biological systems, atmospheric deposition of limiting nutrients can

drive productivity, which affects the fluxes and/or compositions of gases and particles emitted to the atmosphere (Mahowald et al. 2009).

One approach to understanding biosphere-atmosphere interactions is to make a large suite of measurements near to (or within) a major biogenic source of emissions, such as the Amazon rainforest. This permits source signature characterization and studies of the reactivity as emissions are transported away from the source or interact with other atmospheric constituents (see *Reactivity* section below). The GoAmazon project involved a multi-platform field campaign that built upon a longer time series of chemical measurements from a tall tower in the Amazon (Martin et al. 2017). The study sampled both a ‘clean’ biogenic signature from the highly productive rainforest but juxtaposed the biogenic emissions with episodic influence from a major urban area (Manaus, Brazil). The indoor environment bears perhaps unexpected similarity to the GoAmazon study and other forested regions: the building and its contents are major sources of VOCs with their own emissions behavior. Indoor air composition is influenced by the ‘natural background’ of the building, with occupant activity or other time-dependent source behavior (e.g., cooking, cleaning, changes in outdoor air composition and introduction rate) superimposed on top. It becomes clear that a broad view of the building, its behaviors, and chemical signatures is important to gain a more holistic understanding of indoor air quality.

A different approach to understanding a highly complex and coupled system is exemplified by approaches to understanding ocean-atmosphere exchange. The ocean is home to a large and diverse biomass that participates in chemical exchange with the atmosphere. Deposition of inorganic material (e.g., iron, nitrate, phosphate) and uptake of CO<sub>2</sub> provide nutrients for primary production and carbon fixation by microalgae (Emerson and Hedges 2008; Mahowald et al. 2009), but changes in microbiological activity of the near-surface ocean can drive major changes in the water-to-air fluxes of both particles and gases (Wurl et al. 2017; Collins and Grassian 2018). Recognizing the effects of microbial succession on the organic composition of the surface ocean (Prather et al. 2013) has provided key insights into the aerosols and gases that arise from differences in biological activity (Wang et al. 2015; Mayer et al. 2020) that naturally occur on month-long and kilometer scales (Dall’Osto et al. 2019). At the same time, the physical processes that control material fluxes across the air-sea interface occur on the micrometer length scale and involve nuanced (bio)chemistry that occurs in a thin gelatinous film on the ocean surface called the sea surface microlayer (SSML) (Cunliffe and Murrell 2009). Biogeochemical processes occurring within the SSML can be sources of trace gases, but the physical properties of the SSML also physically mediate air-sea gas transfer in both directions (Frew 1997; Wurl et al. 2017). In addition, the air-exposed film may participate in multiphase chemistry, leading to the reactive uptake and/or production of various trace gases (Wurl et al. 2017; Collins and Grassian 2018; Schneider et al. 2019). In the indoor environment, significant effort on the microbiology of the built environment has been initiated (Gilbert and Stephens 2018). Treating the indoor microbiome in a manner analogous to the microbiome of the surface ocean could yield important new insights. It could be important to treat the bi-directional exchange of material on microbially-colonized indoor surfaces with care, as a recent study has shown that the gut microbiome can respond to the chemical environment to which a person is exposed (Gardner et al. 2020). Do bi-directional feedbacks and/or important couplings exist between the microbial communities and the chemistry of the air within a building?

## **Reactivity**

The strength and nature of the sources that supply reactive compounds to the atmosphere impart an important control on the overall amount and type of reactivity observed in the air. Most gaseous and aerosol reactions in the outdoor atmosphere are driven by a cascade of energy from ultraviolet (UV) light in the Sun’s spectrum. Although the most energetic photons are removed in the stratosphere, sunlight with wavelengths in the near UV range penetrate to the ground. Through photochemistry, OH radicals are

formed, which then oxidize VOCs and lead to the formation of O<sub>3</sub> when NO<sub>x</sub> is present. This flow of energy from the Sun also drives nocturnal chemistry, with O<sub>3</sub> formed during the day reacting in the dark with alkenes, also forming radicals (Finlayson-Pitts and Pitts 2000). The implicit approach in atmospheric chemistry is to attempt to define the dispersal of photochemical energy: Which oxidants form? What are their sinks? What oxidation products arise? Large field campaigns are organized around simultaneous, in-situ measurement of short-lived radicals and their precursors along with assessments of radical loss mechanisms (Carlton et al. 2018). Photochemical models, which include representations of fundamental gas-phase chemistry and are constrained by observations from field studies, embody our understanding of the energy cascade from sunlight into more oxidized species.

The same questions arise with the chemistry of aerosol particles and cloud droplets, requiring detailed chemical characterization of the condensed-phase component of the atmosphere. Such multiphase chemistry involves the coupled chemical and mass transfer interactions of atmospheric gases with the surfaces and interior of aerosols, cloud droplets, and ground materials (Ravishankara 1997). In particular, the gaseous products of oxidation reactions may partition to aerosol particles (see *Partitioning* section below), giving rise to secondary aerosol formation. In aqueous aerosol particles and cloud droplets, it is important to evaluate the degree to which condensed-phase oxidants such as H<sub>2</sub>O<sub>2</sub> react with dissolved constituents, giving rise to more oxidized and water-soluble species. This is how one important component of acid rain, sulfuric acid, forms.

We can also track the Sun's input, along with generated oxidants and their impacts, to the indoor environment. Although sunlight penetrates windows, the shortest, most photochemically-active wavelengths are attenuated by glass and the total indoor volume illuminated by direct sunlight is generally low. As well, most indoor lighting is a weak source of UV light (Kowal et al. 2017). As a result, less photochemical energy is available indoors than outdoors and OH radical concentrations are generally low, largely generated by ozone/alkene reactions. Coupled with short indoor air residence times (on the order of hours) (Murray and Burmaster 1995), conditions are not conducive for gaseous reactions to be the primary chemical sink for most indoor contaminants. Ozone is an important low-light oxidant, but is not generated in-situ to a significant degree (Young et al. 2019). While secondary organic aerosol formation can occur in specific situations with high organic precursor and oxidant levels (Waring 2014), the relative contribution of indoor secondary aerosol formation is smaller than the importance of secondary aerosol formation to the total outdoor aerosol mass. Rather, a characteristic feature of indoor environments is that the major flux of photochemically-generated secondary pollutants, such as O<sub>3</sub>, NO<sub>2</sub>, and organic- and sulfate-containing aerosol, is usually associated with introduction of outdoor air. As described above, tracking outdoor-to-indoor transport is a major focus of indoor chemistry and represents a key connection point to outdoor air quality.

With oxidant mixing ratios considerably lower than in outdoor environments, a common misconception is that little oxidation chemistry occurs indoors. In specific situations, gas-phase reactions of ozone with high mixing ratios of terpenes and photolysis of HONO in direct sunlight are important sources of indoor OH (Finlayson-Pitts and Pitts 2000; Gómez Alvarez et al. 2013). As well, ozone mixing ratios are low indoors because so *much* oxidation chemistry is occurring. Just as in outdoor environments, where ozone dry deposits onto reactive surfaces like vegetation, ozone experiences efficient deposition to indoor surfaces with high surface-area-to-volume ratios and which can be coated by reactive surface-sorbed molecules (Morrison 2008), such as unsaturated oils from humans or cooking (Zhou et al. 2019b), or products of incomplete combustion such as polycyclic aromatic hydrocarbons (Zhou et al. 2019a). Whereas the approach of outdoor air pollution research is to focus on the exposure to airborne pollutants by inhalation, it is important to consider indoor exposures based also on human contact with contaminated surfaces, like

dermal uptake or ingestion. The broader spectrum of exposure routes relevant to indoor environments lends importance to understanding the nature of gas-surface multiphase processes.

In the gas phase, an exciting recent finding is the significance for organic molecules of auto-oxidation processes driven by rapid intramolecular isomerizations, giving rise to the formation of highly oxygenated organic molecules (HOMs) (Crouse et al. 2013). Although studied to understand rapid oxidation processes in outdoor environments, even low indoor OH radical and ozone concentrations have the potential to drive the formation of secondary organic aerosol (Kruza et al. 2020). As well, surface-sorbed molecules can react via OH-surface collisions, leading to gradual modification of surface composition over long periods (Alwarda et al. 2018; Morrison et al. 2019).

A distinct and important set of indoor chemical reactions occurs via the use of cleaning agents. The oxidizing capacity of the indoor environment can be amplified significantly in a manner not applicable to outdoor air. Cleaning agents like chlorine bleach and hydrogen peroxide, which are excellent non-specific biological oxidizing agents, are used in large quantities, especially during the COVID-19 pandemic. HOCl, which exists in both the aqueous and gaseous phases during chlorine bleach use, reacts with a wide variety of organic functional groups, including amines, thiols, and carbon-carbon double bonds to form organochlorine products. In addition, HOCl can drive the formation of volatile chloramines and other reactive species when bleach washing is used (Wong et al. 2017; Mattila et al. 2020). H<sub>2</sub>O<sub>2</sub> is also an effective biocide that can photochemically release gas-phase OH when used in large quantities and can also decompose to generate condensed-phase OH radicals on surfaces in the presence of iron.

A challenge to both indoor and outdoor communities is the study of reactions between closed-shell molecules without direct photochemical involvement. High molecular weight organic species form within aerosol particles via condensation reactions between oxygenated organic precursors (Jang et al. 2002). They are likely to also form in highly concentrated organic films like the sea-surface microlayer and are important on indoor surfaces where reaction times are long and reactant surface concentrations can be high. As well, it is known that the ester linkages in surface-bound phthalates can hydrolyze if the pH conditions of the substrates are appropriate (Bope et al. 2019). Such reactions are generally neglected outdoors, given that they are fastest under alkaline conditions.

## **Partitioning**

Determining whether a molecule resides in the gas phase or in an aerosol particle, or is part of a surface reservoir, is of central importance to assessments of human chemical exposure, both indoors and out. Gases can be inhaled but soluble species are scavenged from the breath high in the respiratory tract. Molecules residing in fine particulate matter can reach deep into the lungs before being deposited. Dermal exposure can occur via touching contaminated surfaces or through interactions with contaminants that have partitioned to clothing.

In the outdoor environment, the recent focus on phase partitioning has centered around secondary organic aerosol: the oxidation of VOC precursors leads to the formation of semi-volatile species that can partition to aerosol particles. The HOMs that arise from auto-oxidation processes (see *Reactivity* section above) are frequently of such low volatility that they either undergo one-way condensation to pre-existing particles or to help nucleate new particles (Bianchi et al. 2019). On the other hand, some emissions from the tail pipe of an internal-combustion-engine car are initially part of the particulate exhaust from the car, but then evaporate as dilution occurs downwind of the emission source (Robinson et al. 2007). It is important to describe this highly dynamic environment, with molecules readily moving from the gas phase to aerosol particles and back again.

Recent indoor studies also attempt to capture that dynamic partitioning, illustrated nicely by the impact of third-hand tobacco smoke on indoor air quality. Semi-volatile smoking emissions deposited to indoor walls, furniture, and clothing re-volatilize from these surfaces long after, or far away, from the smoking event (DeCarlo et al. 2018). A striking example is the impact of tobacco smoking on the air quality in a non-smoking movie theatre, where high levels of smoke-derived VOCs are observed in the theatre having been carried inside on the clothing of occupants who previously smoked outside (Sheu et al. 2020). These VOCs can partition to aerosol particles, changing their composition to partly reflect the composition of the third-hand smoke (Collins et al. 2018b).

Gas-surface partitioning behavior is also apparent in indoor spaces when they are ventilated, by opening windows for example. The mixing ratios of most gases, ozone and NO<sub>x</sub> being notable exceptions in most cases, decline because the indoor air is diluted with cleaner air from outside. When the windows are closed, the mixing ratios re-establish steady state levels, reflecting the flux of molecules from indoor surface reservoirs to the gas phase (Collins et al. 2018a; Wang et al. 2020). On the other hand, when excess HONO is added to a house, for example from a gas stove, it is readily taken up by the indoor surface reservoirs (Collins et al. 2018a). Valuable insights into chemical mechanisms can be readily conducted indoors by such perturbation experiments.

A perturbation also arises from the partitioning-dependence of acidic and basic molecules when acidic (i.e. vinegar) or basic (i.e. ammonia) cleaning solutions are used (Wang et al. 2020). Acidic gases that dissociate upon partitioning into polar indoor surface reservoirs are released to a room when vinegar washing proceeds, i.e. the additional acidity shifts the equilibrium state in the surface towards the more volatile, non-dissociated form of the acid. Less water-soluble molecules do not behave in this manner, likely because they are either partitioned into a less polar, more organic-rich surface reservoir or because pH does not affect their volatility.

Outdoors, forced system perturbations are not possible and we rely instead on the natural variability of the environment to provide such information. For example, the flux of ammonia to and from the Earth's surface is dependent on the gas-phase ammonia mixing ratio, the pH of the water in the ground, and the pH of the aerosol in the overlying atmosphere. Such bi-directional flux behavior is only now being incorporated into chemical transport models of the outdoor atmosphere (Whaley et al. 2018; Pleim et al. 2019).

Finally, partitioning to liquid water is a well-known phenomenon in outdoor environments, where water-soluble gases are readily scavenged to cloud water. This is one of the major atmospheric cleansing processes. These lessons are being applied indoors when considering the impact of air conditioning systems on the behavior of water soluble molecules (Duncan et al. 2019; Wang et al. 2020). Liquid water condenses on the cold coils of the air conditioning unit, leading to partitioning of soluble gases. This process is manifest as oscillatory water-soluble gas mixing ratio behavior in the indoor space, as the air conditioning unit that recycles the air turns off and on. There is a direct analogy to clouds: when it rains, water soluble gases are removed from the atmosphere, but cloud droplet evaporation leads to their release back to the gas phase. Likewise, with air conditioning, if sufficient water builds up on the cooling coils that it drains from the unit, then the air inside the house is cleaned somewhat of those species. If the water evaporates instead, those species are returned to the gas phase. In addition to impacts on gas-phase composition, control of indoor environmental conditions also affects aerosol phase state and water content (Cummings et al. 2020).

### **Impact of Dynamics on Chemistry**

Simultaneous production, consumption, phase partitioning, and transport of chemicals in the environment necessitates a broad and multi-faceted approach to realizing an understanding of the system as a whole. Advances in atmospheric chemistry often come through the interplay of field measurements, laboratory



studies, and modeling due to the complex nature of atmospheric chemical processes and their interplay with environmental conditions and the dynamics and structure of the atmosphere (Burkholder et al. 2017).

The atmosphere, while a seemingly continuous fluid medium, has a variety of structural features that control chemistry. Atmospheric boundaries, like zonal boundaries in a building, limit mixing between two parcels of air, but are penetrable on relatively long timescales. Certain chemical processes that may be rapid in one region of the atmosphere, such as catalytic ozone destruction in the stratosphere, are unimportant in other regions. The so-called ‘ozone hole’ in Earth’s stratosphere is a seasonal feature that only becomes apparent when cloud particles are abundant during polar sunrise (Molina et al. 1987; Tolbert et al. 1987) and when a distinct fluid dynamical zone, the polar vortex, restricts mixing with air at lower latitudes (Schoeberl and Hartmann 1991). Still, the halocarbon compounds that lead to catalytic ozone-depletion (Molina and Rowland 1974) are emitted at Earth’s surface and are only capable of reaching the stratosphere because they have atmospheric lifetimes that are much longer than the characteristic mixing time across the tropopause (the boundary that separates the troposphere from the overlying stratosphere). This classic atmospheric chemistry example illustrates the importance of characterizing the chemical environments of different indoor zones by carefully taking into account the sources, chemistry, transport, and the importance of different phases to a given phenomenon.

Recent studies using real-time measurements of trace gases have illustrated the level of control that transport dynamics and the boundary structure within buildings have on the composition of indoor air. Space- and time-resolved measurements of inhabited buildings (e.g., residences, schools, and offices) require sophisticated instrumentation, broad access to the building for scientists, and careful collection of metadata, but can yield important results and information about the impact of indoor activities and building structure on indoor air quality. A notable study using a residence across multiple seasons employed a chemical tracer approach to understand and quantify transport between zones (Liu et al. 2018). The *route* of air exchange between the indoors and outdoors may be important to consider and may include a variety of parallel paths including transit through other zones of the building. Such behavior may have important implications for the chemicals that can be lost from, or entrained within, the air as it moves from outdoors to indoors; physical and chemical aspects of the building itself may have important and non-intuitive impacts on the chemistry that drives indoor air quality.

Modeling the interplay of chemistry and dynamics in the outdoor atmosphere is often performed on a variety of spatial scales: from full global simulations down to detailed regional models, and then even further down to simulate the detailed physics of single clouds, for instance. The level of detail in a large-scale model is necessarily coarse and becomes generally more sophisticated as the model scale becomes smaller. Gas phase chemistry can be simulated in roughly any pixel or grid cell size with the assumption that the grid cell is homogeneously mixed. Using this ‘well mixed’ assumption, box modeling has proven useful for a variety of indoor chemistry scenarios for the last few decades. Exciting results from computational fluid dynamics (CFD) models that include chemical mechanisms are beginning to show interesting and important chemical gradients within a single building zone (Won et al. 2019, 2020). Spatially-resolved chemical measurements of air within a room could be designed to couple with CFD modeling. Process-level chemical models may be nested within the CFD simulations or could be parameterized to reduce computational expense. Efforts to reduce computational cost has enabled major advancements in atmospheric and chemical modeling. Collaboration between computational scientists (Shiraiwa et al. 2019) will help to translate indoor measurements and process-level studies into actionable outcomes and should strive to produce new computational tools to advance the practice of producing and maintaining healthy environments within buildings.

## **Working Toward Solutions**

Collaboration amongst experts in diverse fields of engineering, chemistry, biology, public policy, building science, public health, and others will be required to grasp the breadth of interactions that influence indoor air quality and to devise methods for optimizing the living and working environment where many people spend the majority of their lives. Outdoor atmospheric chemistry issues that represent degraded environmental conditions (e.g., acid rain, stratospheric ozone depletion, urban pollution) have been addressed through broad public policy actions such as the international Montreal Protocol on Substances that Deplete the Ozone Layer or the Clean Air Act in the United States. Indoor air quality, however, is subject to weaker government regulation and has been mostly addressed by concerned homeowners or private institutions. A commercial indoor air quality industry has thus emerged to enable private mitigation actions to take place. Outdoor air quality issues include important aspects of environmental justice, as poor air quality disproportionately affects impoverished and non-white communities (Mikati et al. 2018). Health risks due to ambient airborne particulate matter pollution exposure are decreasing in wealthier regions and increasing in poorer regions worldwide (Murray et al. 2020). Since people spend a dominant fraction of their time indoors (Klepeis et al. 2001), a large portion of unhealthy outdoor air is actually breathed while inside the home. Housing quality has also been shown to have a relationship with rates of asthma and other chronic diseases, specifically among urban public housing inhabitants (Digenis-Bury et al. 2008; Northridge et al. 2010), where poor indoor environmental quality can compound negative effects of outdoor air quality. The comparatively weak ability of poorer groups living in nations with highly developed economies, along with large swaths of people in nations with still developing economies, to implement adaptations to our changing climate will exacerbate inequalities in housing and indoor air quality (Islam and Winkel 2017). The commercialization and private-responsibility that has been built into improving indoor air quality has the potential to multiply existing environmental inequalities as groups of people with low access to financial resources may not have the means or the opportunity to implement engineering solutions or retrofits that mitigate degraded indoor air quality (Northridge et al. 2010). As experts and practitioners of air quality studies and solutions, we must acknowledge and work against structural inequality from our own perspectives and positions of power.

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