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Quantifying ambient concentration and emission profile of D5-siloxane of a residential neighborhood in the Greater Houston area†

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Volatile chemical products (VCPs) in urban environments account for a significant portion of the volatile organic compounds (VOCs), enhancing the production of tropospheric ozone and secondary organic aerosols. Residential areas are an important source of VCPs in the urban environment, though few studies have examined the emission of VCPs in metropolitan areas from subtropical regions. To bridge the knowledge gap, this study aims to analyze the concentration and emission of D5-siloxane, a compound typically served as a tracer to characterize VCP emission from residential areas. The Texas A&M mobile laboratory, equipped with a Vocus 2R Chemical Ionization Mass Spectrometer (CIMS), and other gas and particle analyzers, continuously sampled the ambient gas phase concentration of D5-siloxane during a field deployment in a residential neighborhood near Houston, TX. A 0-D box model combining Planetary Boundary Layer Height (PBL) height, hourly D5-siloxane concentration, gas deposition velocities, and D5-siloxane reaction rate with hydroxyl radicals was constructed to represent emissions during our sampling period to derive the emission intensities of D5-siloxane. Monte Carlo statistical analysis was performed to gain insights into the emission profile of D5-siloxane, showing higher emission rates compared with other cities in North America but comparable to emissions of European cities. This study presents time-series concentrations and emissions of D5-siloxane in a subtropical residential area during the wintertime. The findings illustrate the temporal profile of D5-siloxane in a typical residential neighborhood in the Southeast United States and provide valuable data to enhance model parameterizations.

Environmental significance

Volatile chemical products (VCPs), a subset of volatile organic compounds from non-tailpipe emissions, play an ever-increasing role in urban and suburban ozone formation. D5-siloxane, a major VCP product from personal care products, often serve as a tracer for VCPs in residential area and affect regional air quality. Previous studies have primarily focused on quantifying D5-siloxane in temperate climate regions, leaving a gap in understanding its concentrations and emission profiles in subtropical metropolitan areas. This limitation hinders accurate predictions regarding the concentrations and air quality impacts of volatile chemical products (VCPs) in such regions. This study presents the first real-time mass spectrometry data from the Greater Houston Area, aiming to not only ascertain concentrations of D5-siloxane in a subtropical city, but to also model the per-person emission of D5-siloxane in one of the United States' largest metropolitan areas. The derived emission results in the Southeastern United States will allow for significant and deeper understanding of the concentration and air quality impacts of VCPs in similar climate zones globally.

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1. Introduction

Volatile chemical products (VCPs) are emerging volatile organic compounds (VOCs) that are emitted from residential and industrial sources, such as pesticides, coatings, cleaning agents, and other chemical products.[1] The high emission factors and ambient concentrations of VCPs in urban areas raise concern for how these compounds affect local ozone and secondary organic aerosol formation.[2–5] Due to the decrease in emissions of VOCs from combustion sources in the United States,[6] the necessity of understanding VCP contributions to air quality has grown significantly.[7] Personal care products can make up to 25% of the total emission value of VCPs.[8] D5-siloxane, a major component of the personal care products,[9] often shows relatively high concentrations in residential areas and therefore often serve as a trace for residential VCP emissions.[10] In addition, the oxidation products of D5-siloxane have longer atmospheric lifetimes, ranging between 3.5 to 7 days outdoors, potentially contributing to prolonged influence on air quality in urban and suburban areas.[11–16] D5-siloxane is also considered bioaccumulative and toxic to humans, based on studies performed on animals.[17–21] Due to these negative effects associated with D5-siloxane, the EU has moved to require concentrations of D5-siloxane in products to be less than 0.1%, highlighting the importance of understanding its emission and atmospheric concentration.[22]

Historically, outdoor measurements of D5-siloxane are relatively limited. The majority of studies aimed to quantify ambient concentrations in urban or downtown locations of metropolitans areas,[15,23–27] while other studies focused on interior measurements and modeling of D5-siloxane.[28–30] Studies examining the concentrations of ambient D5-siloxane were either in Europe or the Northern United States.[24,31] For instance, Yucuis et. al. measured ambient concentrations of cyclic siloxanes in Chicago and a few Iowa cities.[23] Coggon et al. measured emission patterns of D5-siloxane in Boulder, USA and Toronto, Canada.[5] These studies demonstrate that D5-siloxane has distinct diurnal patterns in major cities, often peaking in the morning time, with a smaller increase near the early evening.[23,32] In addition, Coggon et.al. also shows that D5-siloxane is correlated with traffic emissions, with elevated D5-siloxane/benzene ratios being over 0.3.[32] The concentrations of D5-siloxane were often in excess of 140 ng m^{-3} in previous work,[15] with emissions per person ranging between 100–420 mg per person per day.[31] Notably, a peak emission of 690 mg per person per day was documented in Zurich in winter,[24] a densely populated European city.

To date, all major studies on D5-siloxane have occurred in the upper-mid latitudes,[15,23–27,31] leading to relatively poor characterization of D5-siloxane in the subtropical region, including the Southeastern U.S. region. Given that the atmospheric conditions and population densities in the Southeastern US can be drastically different than previously studied locations,[33–36] understanding the emission profile of D5-siloxane in the Southeast US is necessary for furthering the understanding of the impact of D5-siloxane on ozone and

particulate matter in this region with strong photochemical reaction potentials.[24,31,32,36] Since 1991, the average annual in the Southeast US is roughly 12–18 °F warmer than Chicago and roughly 7–10 °F warmer than Iowa, where D-5 siloxane concentrations were previously reported.[36] Along with temperatures, the Southeast US receives on average 20–30 inches more of rainfall than Chicago annually, and 10–20 inches more of rainfall than Iowa annually since 1991.[36] The higher temperature in the Southeast U.S. may increase D5-siloxane concentrations, which have been found to be positively correlated with temperature, and in some cases, humidity.[37] In addition to these climatological differences, geographical differences are also present in previous studies. Most of the Southeastern US has coastline or is in near proximity to either the Gulf of Mexico or the Atlantic Ocean. This results in heavy marine air mass influence,[34] with sea breezes constantly influencing the movement of air masses,[38] reducing the mixing ratios of pollutants due to horizontal advection.[39] On the contrary, Chicago only has influence from the Great Lakes, and Iowa is landlocked and thus is generally unaffected by marine air mass changes as usually only continental air masses are positioned over these areas.[34] The population distributions also differ between these locations.[35] The Northeastern United States has denser pockets of population as opposed to the Southeastern United States, which has more spread-out urban areas surrounded by larger sections of rural areas.[35] Such differences in population distributions could also contribute to differences in emission profiles and need to be addressed in model parametrizations from ambient measurements. The Houston area is dominated mostly by maritime tropical (mT) air masses,[33,34] making its weather patterns and climate similar to the rest of the Southeast United States.[36] A field study conducted in the suburban area of Houston allows for the characterization of D5-siloxane emissions in a major metropolitan area for the Southeast United States.

In this research, the ambient concentration of D5-siloxane was reported in a residential neighborhood in the Greater Houston Area in winter 2023 using a Vocus 2R chemical ionization mass spectrometer (CIMS). Emission factors of D5-siloxane were derived using modeled and measured meteorological conditions, oxidation precursor concentrations, and concentrations of D5-siloxane. The per capita emission factors of D5-siloxane over the sampling period were compared with emissions from other locations, demonstrating a distinctive profile in the Southeastern U.S.

2. Materials and methods

2.1 Instrument and data collection

2.1.1 Vocus 2R CIMS calibration. The Texas A&M Mobile laboratory was equipped with a Vocus 2R Chemical Ionization Mass Spectrometer (CIMS), as well as other gas and particle analyzers, as shown in the schematics of the mobile lab in Fig. 1. The Vocus 2R CIMS was run in proton transfer reaction (PTR) mode for the entirety of the collection period from January 26th–29th.[40,41] Albeit relatively short, the sampling period captures both several weekdays and a weekend as well as

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a dynamic shift of weather pattern, providing potential examples in the differences in concentration of D5-siloxane, a gas directly related to personal care product use, under different meteorological and population conditions. The real-time measurements that the Vocus 2R CIMS provides provide a next level insight into the hourly changes in D5-siloxane during the day and overnight. Future work covering a longer sampling period is desirable to provide more statistically robust information regarding the concentrations and emissions of D5-siloxane. Herein we refer to January 26th–29th as Days 0–3. Every 6 hours, a calibration was performed using a mixture of calibration gases that included the target gas, D5-siloxane, with the concentration of D5-siloxane being 973 ± 49 ppb. These calibrations were conducted to quantify the sensitivity of the Vocus 2R CIMS to D5-siloxane specifically over time, improving the accurate quantification of ambient D5-siloxane mixing ratios. By assessing the calibration factors produced in Table S1,† the response of the Vocus to environmental factors, specifically temperature,[42] can be mitigated, potentially interfering compounds can be mitigated, and mixing ratios of D5-siloxane can be accurately quantified. The limit of detection for D5-siloxane was 2.2 ppt, determined by three times the standard deviation of background signal over thirty seconds of integration. This is in agreement with another study, which places the LOD at 1 ppt.[43] During these calibrations, the main Vocus inlet was automatically closed, and zero air (N_2) was introduced into the Vocus at a flow rate of 300 standard cubic centimeters per minute (sccm) for 2 minutes. After these two minutes, the calibration gas was introduced into the Vocus at a flow rate of 5 sccm, with the zero air still on to provide dilution, reaching a calibrant concentration of 15.9 ± 0.8 ppb. The calibration gas remained on until the signal from each of the gases within our calibration gas stabilized for at least 1 minute. After the signals of the calibrants stabilized, the calibration gas was left on for another minute, and then turned off along with the zero air. The Vocus ambient inlet was re-opened, ending the calibration. Our calibration gas is NIST calibrated, and is diluted and directly flown into the Vocus, imitating ambient sampling. The Vocus 2R, which is our model, also has a specified mass resolving power of over 15 000 $m/\Delta m$, alleviating interference from nearby signals to D5-siloxane.[44] Our calibration method is similar to other Vocus measurements, which decreases the effect of external and internal variations as well as uncertainty.

2.2.1 Population data. The location of the measurement site was a residential suburban single-family house in the
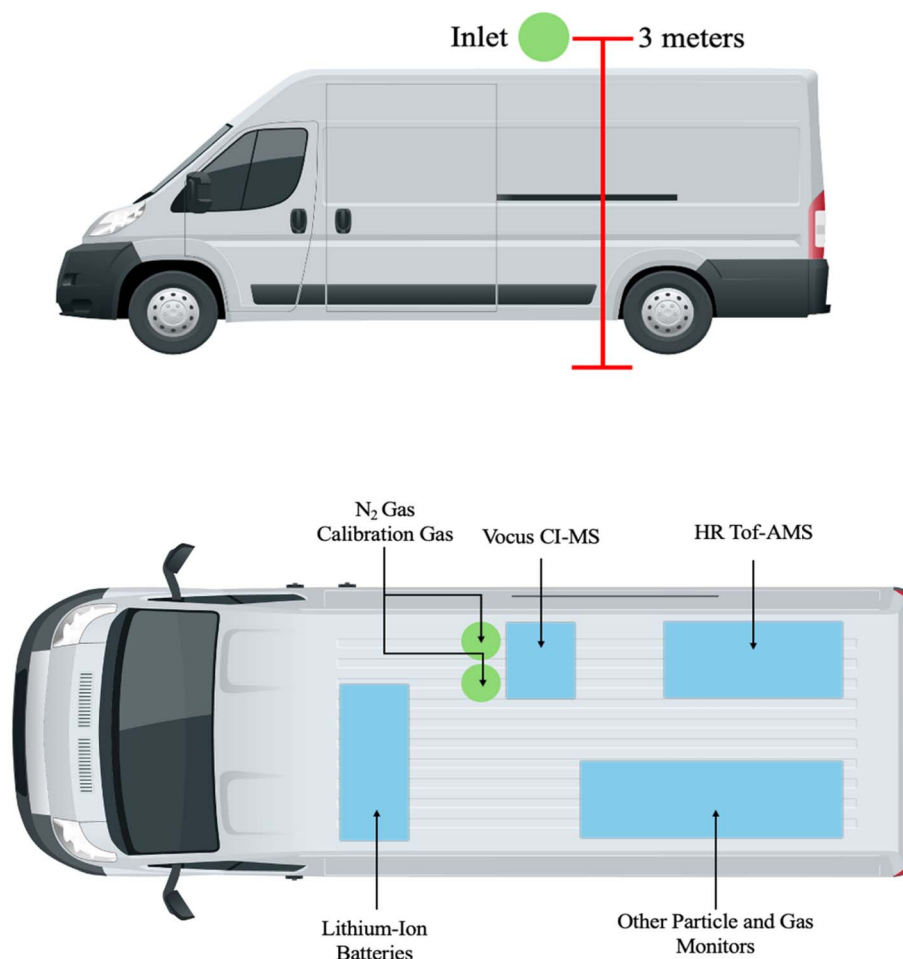

Fig. 1 Schematic of the Texas A&M Mobile Lab setup, showing the location of the inlet, Vocus, and other instruments.

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neighborhood of Cane Island, located in West Houston, 53 kilometers from the center of Houston. The location of the sampling site in relation to the rest of Houston is shown in Fig. 2. This neighborhood is rapidly growing, and is highly representative of a suburb of Houston, with houses that share fence lines but population density lower than that of an urban population density. The location of the measurement site reduces the fluctuation of population from office buildings and the influence of VCP emissions from inner city Houston and the ship channel.[45] It is worth noting that Houston is a rapidly developing area, therefore the most recent US census from 2020 does not accurately represent the population of the area sampled. To accurately quantify population density, the closest available Google Earth Imagery from June 2023 was employed, and individual houses within 1, 2 and 3 km² area circles of the collection site were counted,[46] as shown in Fig. 2. There were 378 total houses in the 1 km² area, 783 total houses in the 2 km² area, and 1041 total houses in the 3 km² area. Each subsequent area included the previous sections' house count in the total count. These counted houses were then multiplied by the assumed average number of people per household in the US (2.51), to produce an estimate of the population within these marked zones.[47] It is worth noting that an elementary school is located within the 1 km² circle. Given a portion of the students do not live within the marked circle areas as shown in Fig. 2, the influence of this school on the local population needs to be accounted for. However, elementary schoolers do not tend to wear personal care products that emit D5-siloxane, so only teachers and parents that enter the area to drop off and pick up their students should be accounted for in per capita emission calculation. In order to account for this, population ranges from 949 to 1249 for 1 km², 1959 to 2259 for 2 km², and 2612 to 2912 for 3 km² were created using the enrollment of the elementary school[48] and the pre-existing counted population data during weekdays. These ranges were created by ranging the population from zero school influence to half of the total enrollment of the elementary school (roughly 300 students). On weekends, this population change was not included due to the closure of the school.

2.2 0-D box model

This 0-D box model takes measured and modeled inputs to quantify daily emission estimation using chemical reaction rates and meteorological conditions. A schematic of the interactions between terms in the box model is represented in Fig. S1.† Eqn (1) describes the concentration change of the gas molecule of interest from sources and sinks.[49]

$$\frac{dC}{dt} = -k_i \times [OH]_i \times C_i - \frac{\nu_{d_i}}{H_i} \times C_i + \frac{E_i}{H_i} + \frac{1}{H_i}$$
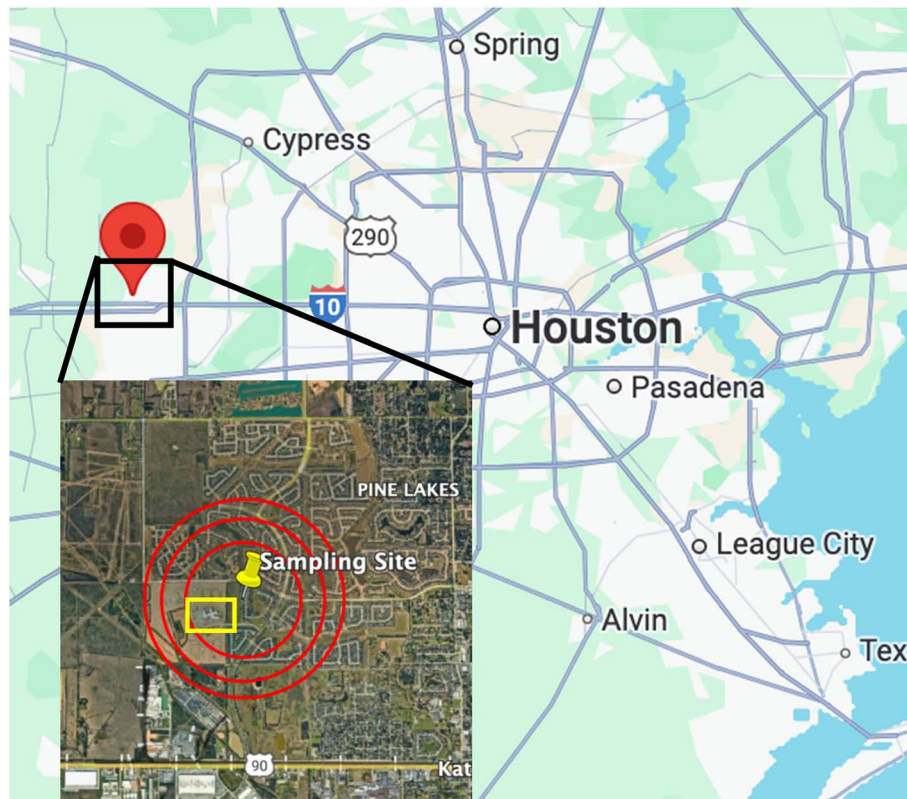$$\times \frac{H_{i+1} - H_i}{\Delta t_i} \times (C_{b_i} - C_i) \tag{1}$$

Fig. 2 Location of the sampling site in relation to the Greater Houston Area. Zoomed in is the marked areas where the model accuracy for different population groups and areas was assessed. Boxed in yellow is the elementary school, and the red circles represent the 1, 2, and 3 km² areas.

The term C is measured concentration of D5-siloxane, k is the reaction rate of D5-siloxane with OH radicals, [OH] is the concentration of OH radicals, ν_d is the gas deposition rate of D5-siloxane, H is the mixing layer height, E is emissions, C_b is the vertical background concentration of D5-siloxane. Eqn (1) is then rearranged to solve for emissions, as shown in eqn (2).

$$E_i = H_i \times \frac{(C_{i+1} - C_i)}{\Delta t_i} + H_i \times k_i \times [OH]_i$$
$$\times C_i + \nu_{d_i} \times \; C_i - \frac{H_{i+1} - H_i}{\Delta t_i} \times (C_{b_i} - C_i) \quad (2)$$

The concentration used in the model is taken from ambient D5-siloxane measurements with the Vocus 2R CIMS. The reaction rate of D5-siloxane was obtained from Atkinson *et al.* with a value of $(1.55 \pm 0.17) \times 10^{-12}$ cm³ per molecules per s.[50] Hydroxyl radical concentration and the gas deposition rate was obtained from the CMAQ Model version 5.0.1.[51] The PBL height was obtained from the WRF model.[52] This PBL height data was also compared with model outputs from the ERA 5 Reanalysis,[53] showing agreement in trend for PBL on each day. Background concentrations of D5-siloxane were also obtained from the CMAQ model, representing concentrations above the mixing layer.[51] Attempting to include a horizontal transport term in the model proved challenging, as modeling surface concentrations of D5-siloxane for a background concentration value proved outside the scope of this model, and winds during the sampling period were calm and locally variable. It is worth noting that the model is unable to account for extraneous interference to D5-siloxane concentrations, such as secondary or tertiary reactions within the atmosphere or slight changes in meteorology that affect both boundary layer height and gas deposition velocity. In order to account for these uncertainties, if not specified, the parameters in the model include a 20% uncertainty. This uncertainty, although on the larger side, allows for the capture of a valid mean and valid standard deviation for D5-siloxane emission within our 10 000-point emission Gaussian distributions. We also note that D5-siloxane can react with chlorine atoms in the atmosphere, but parameterizing this was outside the scope of this study.[54] Daily plots of each term are shown in Fig. S2–S4.† Emissions are in the unit of milligrams per person per day.

2.3 Data analysis method

2.3.1 Concentration calculation.
In order to accurately derive the concentration of D5-siloxane from the Vocus 2R CIMS data, Tofware software that runs on Igor Pro. (Wavemetrics, Inc.). was used.[55] The m/z calibration and peak fitting were conducted in order to accurately derive counts per second (cps) of D5-siloxane.[55] After counts per second (cps) time series of each of the targeted gases were obtained, the mixing ratios were then calculated using the instrument sensitivity to the gas derived from the calibration in Section 2.1.1. The mean ion count of each stable calibration period was plotted against the concentration of the calibration gas, with the slope being the ion sensitivity (cps per ppb). The calibration factors (cps per

ppb) at each calibration point for D5-siloxane are shown in Table S1.† Using these sensitivities derived at each point, linear interpolation was performed to obtain the assumed sensitivity of the Vocus 2R CIMS at each sampling point. The mixing ratios of D5-siloxane were obtained with the cps data and the derived sensitivities.

2.3.2 Emission calculations and error propagation.
Eqn (2) contains multiple variables that have different uncertainty ranges. To constrain the uncertainty of the emission value derived from eqn (2), the Monte Carlo statistical analysis method was employed. A 10 000-point normal Gaussian distribution representing each parameter of eqn (2) was created, with the standard deviation and mean being assigned the same as the sampled data. An example of these 10 000-point normal Gaussian distributions can be seen in Fig. S5.† For instance, the standard deviation of D5-siloxane measurement using the Vocus 2R CI-MS (C_i in eqn (2)) is estimated by eqn (3).[56]

$$\sigma_{signal} = uncertainty \times \sqrt{signal} \quad (3)$$

The mean value of each distribution was assigned to each parameter in eqn (2) to calculate the emission intensity. The mean of the emission distribution represents the averaged emission value, with the standard deviation of the distribution being the error associated with the emission value from that hour. Only half of the data is available on Day 3, hence the emission profile from the previous day was used to characterize the total emission, as both are on the weekend and the meteorological conditions are similar. The fraction of emissions between 12 am and 10:59 am local time was 59% of the whole day for the previous day, therefore, this value was applied to estimate the whole-day emission of Day 3.

Eqn (2) uses Planetary Boundary Layer (PBL) height to represent the mixing layer.[57] In wintertime, shallow surface temperature inversions would inhibit the mixing of surface-emitted D5-siloxane to the planetary boundary layer.[58] To reduce the uncertainty in mixing layer height, meteorological analyses of Skew-Temperature Log-Pressure (Skew-T Log-P) diagrams produced by the High-Resolution Rapid Refresh Model (HRRR) were used to determine temperature inversions near the surface.[59] The hourly model runs are the 0 hours runs, which ingest previous radar, satellite, and sounding data to produce temperature profiles.[59] The conditions derived from the HRRR model often closely represent actual measurement data by a weather balloon launched from the surface at the current hour.[59] These soundings were obtained using the Python-based program SHARPy.[60] The 0 hours model runs for every hour are shown in Fig. S6–S10.† Based on the determination of a surface inversion layer from the HRRR Skew-T Log P diagrams, the surface mixing height in eqn (2) was then adjusted between 0.4 and 0.5 of the original modeled PBL height to obtain a better representation of surface-based observations, given the sampling height is only 3 meters off the ground. The adjustment of PBL height accounts for estimated surface inversions, and the range allows for analysis of imprecisions in methodology for this mixing layer

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determination. The adjustment values are based on estimations of inversion layer heights from the Skew-T Log P diagrams. This methodology is similar to what was described in Buser *et.al.* 2013, which adjusted mixing layer height based on meteorological conditions in Switzerland by analyzing potential temperature.[24] All of the above analyses were conducted using Python 3.8.10, with the packages NumPy 1.21.2, matplotlib 3.5.2, pandas 1.3.2, and xarray 0.19.0.[61–64]

3. Results and discussion

3.1 Measured ambient D5-siloxane concentration

The full sampling period concentrations of D5-siloxane are shown in Fig. 3. A rolling window average was conducted in order to alleviate the effect of inter-hour deviations but still capture the overall D5-siloxane concentration trend. During the sampling periods, the concentration of D5-siloxane ranged between 5 and 25 parts per trillion (ppt), with an average concentration of 23 ± 2 ppt. It is worth noting that there were day-to-day variations of D5, with a spike of concentration on Day 1, peaking over 120 ppt. Ambient concentrations in this residential area in Houston are similar to measurements in Toronto and Boulder, generally ranging from 5 to 30 ppt, with spikes above this range occurring occasionally.[32] Peak concentrations in Toronto were found to be over 60 ppt.[32] Similar results are also found in Zurich, with concentrations ranging between 5 and 20 ppt.[24] On Days 2–3, the peak concentrations were less than on Day 1, likely attributed to these days being Saturday and Sunday and less of the population leaving their homes. Applying hourly measured concentrations to the in-house 0-D box model described in Section 2.2, we calculated the emission profiles of one weekday and two weekend days. These emission profiles are described in the upcoming sections.

3.2 Weekday emission profile

The emission results for D5-siloxane on Day 1 (Friday) calculate in the ranges of 400–654 mg per person per day. These emission

Table 1 The per capita emissions ranges derived from this study during each of the sampling day

Day	Per capita emission ranges (mg per person per day)
Day 1, Friday	400–654 mg per person per day
Day 2, Saturday	189–271 mg per person per day
Day 3, Sunday	160–208 mg per person per day

results are shown in Table 1. Peak emissions occurred throughout the morning, which was to be expected as the local population likely leaving their homes. In addition, the morning period was when parents and teachers arrived at the school that was close to the sampling site, further enhancing the local emissions of D5-siloxane in the area. Another spike, although not as large, occurred in the evening, and was attributed to the return of the local population from work, as well as Friday evening activities. The emission results are in the upper bounds and slightly higher than those reported by Buser *et al.* 2014 in Chicago, showing general D5-siloxane emission rates between 100-420 mg per person per day.[31] The emission of D5-siloxane in this location was also above the average emission of 310 mg per person per day measured in Zurich, Switzerland over 7 days, although daily values was lower than the maximum D5-siloxane emissions of 690 mg per person per day during an inversion process.[24] Such results suggest that the emission of D5-siloxane in Houston is potentially higher than in other Northern U.S. and European cities. The difference in sampling methodology and focus between studies may also may play a role in the elevated results for Houston, as our study was specifically limited to a residential neighborhood as opposed to an entire city.[23,24] We refer back to the discussion in the introduction about climatological differences between our sampling location and other studies' sampling locations. We believe that differences in weather features contributes, but is not solely responsible for, the differences in D5-siloxane emissions between sampling locations. D5-siloxane from personal care products evaporates off of surfaces faster in higher temperatures,[65] which is why we
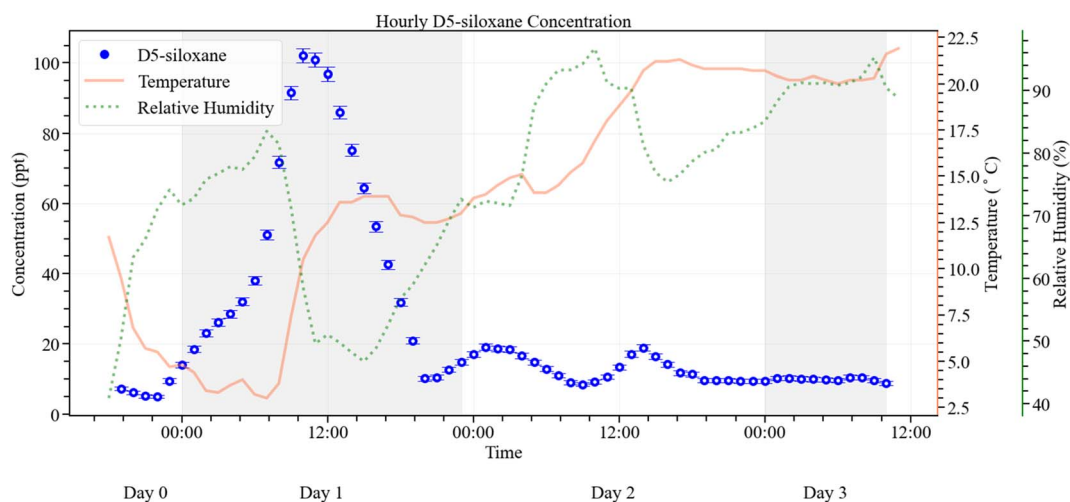

Fig. 3 Measurements of D5-siloxane ($C_{10}H_{30}O_5Si_5$) concentration, surface temperature, and relative humidity throughout the sampling period. Shaded and light areas represent different days.

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highlight the importance of differing regional climatology. Regardless, future measurements in more subtropical metropolitan areas may be needed.

3.3 Weekend emission profiles

The diurnal emissions of D5-siloxane from our box model for Days 2–3, representing Saturday and Sunday, are also shown in Table 1. These emission rates lie in the range in Buser *et al.* 2014 of 100–420 mg per person per day.[31] On Day 2, subtracting the population attributed to the school due to the weekend, emissions ranged from 189–271 mg per person per day. For Day 3, the emissions ranged from 160–208 mg per person per day. For the entire weekend, the average emission value is 207 ± 47 mg per person per day. Both these days exhibited a smaller per capita emission range than Day 1. This difference can be attributed to less population influx due to the school being closed on weekends, and fewer people working on the weekends, leading to less usage of personal care products or being outside of their homes. A D5-siloxane study from New York City compared to other studies finds a positive correlation with an R^2 of 0.59 with population,[66] following with our measurements and changes in local population between a weekday and a weekend. In Houston, public schools are open Monday through Friday and closed on the weekend, and students that do live outside the neighborhood are still zoned to the elementary school they attend on weekdays. A map of the area zoned to the local elementary is included in SI Fig. 11.†[48] All of the per person per day emission values are shown in Table 1.

3.4 Discussion

Our box model can effectively provide a range of values for the emission of D5-siloxane in a suburban residential area in Houston. Over the whole period of measurements, the emission rate of D5-siloxane ranges between 160–654 mg per person per day with an average rate of 412 ± 177 mg per person per day. This average value is more than 100% higher than the average emission range of Chicago, and ~30% higher than the average emission of D5-siloxane in Zurich in winter,[31] highlighting the importance of geographical differences and personal habits in affecting the D5-siloxane emissions.[31] Although not much data on personal care product usage in relation to climatologically different regions is available, one survey finds that the southern US has a higher use rate of deodorant/antiperspirant on a daily basis than other defined regions, being the Midwest, northeast, and west.[67] Comparisons between the emissions obtained from this study with previous studies are shown in Fig. 4. Based on our emission results being elevated compared to previous studies,[24,31] these results show that the emission of D5-siloxane may not be even distributed within cities or downtown areas, with "hot spots" of D5-siloxane occurring over other populated areas such as residential neighborhood or schools. Such hot spots would in turn result in underestimating potential ozone production in emission inventories, due to the ability of D5-siloxane to enhance ozone production.[5] This means that in residential areas, ozone concentrations could be elevated when higher D5-siloxane concentrations occur, holding all other parameters constant. Ozone production in Houston is VOC-limited, and so increased VCP concentrations results in the increase in ozone production.[68] It is also worth noting that based on wind direction on the 27th, an air mass change is indicated based on flow direction changing from northerly to southerly, resulting in oceanic air cleaning out the D5-siloxane over the neighborhood. This pollutant reduction is seen in the D5-siloxane concentration time series in Fig. 3. This is in
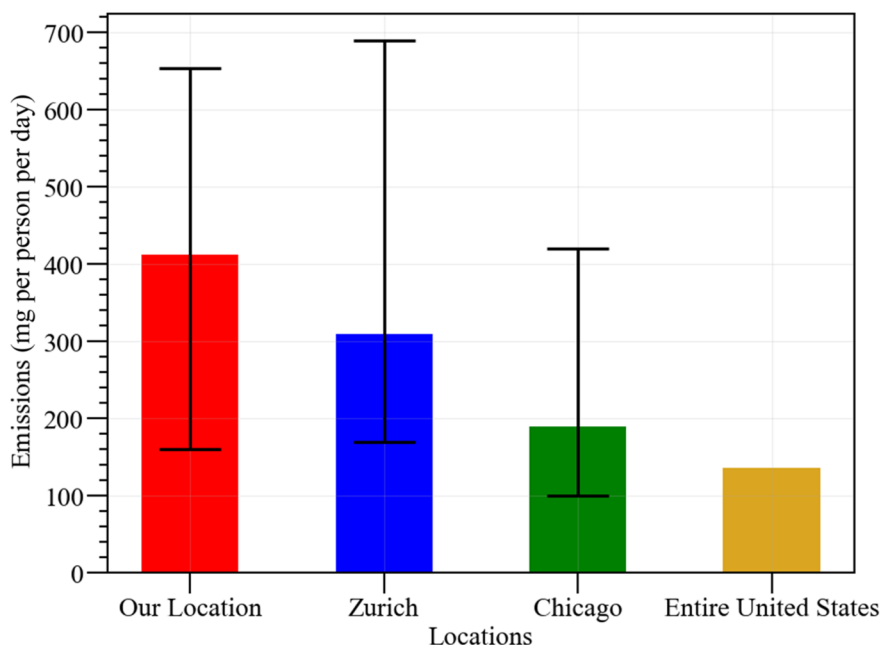

Fig. 4 The estimated D5-siloxane emissions from our site, Zurich (Buser *et al.* 2013),[24] Chicago (Buser *et al.* 2014),[31] and the entire United States (Navea *et al.*).[69] The black uncertainty bars are the estimated emission ranges from this study and previous research.

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agreement with the idea of the modulation of local coastal air quality by the ocean.[39] The changes in wind direction observed are shown in Fig. S12.†

Besides providing the averaged emission rates of D5-siloxane in a suburban area in the Southeastern U.S., this study also shows that the emission might demonstrate weekday-weekend effects. The emission was less on Day 2–3 due to weekend effects, as the school did not operate, and less of the population commuted to work. More studies need to be conducted to further analyze the difference between weekday and weekend emission profiles in suburban environments.

Overall, this work provides the emission profile of D5-siloxane in a residential area in one of the largest U.S. cities in the Southeastern U.S. The reported higher per capita emission values allow for the enhancement of modeling of D5-siloxane in the southeast US, as well as provide further insight into updating emission inventories. In addition, understanding the emission pattern of D5-siloxane in suburban residential areas contributes to determining how personal care products and other chemical products can lead to outdoor air pollution, especially for residents in suburban areas. Future work with longer sampling periods, in different seasons, and in other regions will allow for a better understanding of emission profiles of D5-siloxane in the residential environment.

Data availability

The data used in this article, including raw measurements of D5-siloxane, relative humidity (RH), and temperature, are publicly available on the Open Science Foundation. The data are listed in a time-series format and can be accessible at https://doi.org/10.17605/OSF.IO/PG2AW.

Conflicts of interest

There are no conflicts to declare.

Acknowledgements

References

1 M. Qin, B. N. Murphy, K. K. Isaacs, B. C. McDonald, Q. Lu, S. A. McKeen, L. Koval, A. L. Robinson, C. Efstathiou, C. Allen and H. O. T. Pye, Criteria pollutant impacts of volatile chemical products informed by near-field modelling, *Nat Sustainability*, 2021, **4**, 129–137.

2 G. I. Gkatzelis, M. M. Coggon, B. C. McDonald, J. Peischl, K. C. Aikin, J. B. Gilman, M. Trainer and C. Warneke, Identifying Volatile Chemical Product Tracer Compounds in U.S. Cities, *Environ. Sci. Technol.*, 2021, **55**, 188–199.

3 J. L. Jimenez, M. R. Canagaratna, N. M. Donahue, A. S. H. Prevot, Q. Zhang, J. H. Kroll, P. F. DeCarlo, J. D. Allan, H. Coe, N. L. Ng, A. C. Aiken, K. S. Docherty, I. M. Ulbrich, A. P. Grieshop, A. L. Robinson, J. Duplissy, J. D. Smith, K. R. Wilson, V. A. Lanz, C. Hueglin, Y. L. Sun, J. Tian, A. Laaksonen, T. Raatikainen, J. Rautiainen, P. Vaattovaara, M. Ehn, M. Kulmala, J. M. Tomlinson, D. R. Collins, M. J. Cubison, E. J. Dunlea, J. A. Huffman, T. B. Onasch, M. R. Alfarra, P. I. Williams, K. Bower, Y. Kondo, J. Schneider, F. Drewnick, S. Borrmann, S. Weimer, K. Demerjian, D. Salcedo, L. Cottrell, R. Griffin, A. Takami, T. Miyoshi, S. Hatakeyama, A. Shimono, J. Y. Sun, Y. M. Zhang, K. Dzepina, J. R. Kimmel, D. Sueper, J. T. Jayne, S. C. Herndon, A. M. Trimborn, L. R. Williams, E. C. Wood, A. M. Middlebrook, C. E. Kolb, U. Baltensperger and D. R. Worsnop, Evolution of Organic Aerosols in the Atmosphere, *Science*, 2009, **326**, 1525–1529.

4 B. C. McDonald, J. A. de Gouw, J. B. Gilman, S. H. Jathar, A. Akherati, C. D. Cappa, J. L. Jimenez, J. Lee-Taylor, P. L. Hayes, S. A. McKeen, Y. Y. Cui, S.-W. Kim, D. R. Gentner, G. Isaacman-VanWertz, A. H. Goldstein, R. A. Harley, G. J. Frost, J. M. Roberts, T. B. Ryerson and M. Trainer, Volatile chemical products emerging as largest petrochemical source of urban organic emissions, *Science*, 2018, **359**, 760–764.

5 M. M. Coggon, G. I. Gkatzelis, B. C. McDonald, J. B. Gilman, R. H. Schwantes, N. Abuhassan, K. C. Aikin, M. F. Arend, T. A. Berkoff, S. S. Brown, T. L. Campos, R. R. Dickerson, G. Gronoff, J. F. Hurley, G. Isaacman-VanWertz, A. R. Koss, M. Li, S. A. McKeen, F. Moshary, J. Peischl, V. Pospisilova, X. Ren, A. Wilson, Y. Wu, M. Trainer and C. Warneke, Volatile chemical product emissions enhance ozone and modulate urban chemistry, *Proc. Natl. Acad. Sci. U. S. A.*, 2021, **118**, e2026653118.

6 B. C. McDonald, D. R. Gentner, A. H. Goldstein and R. A. Harley, Long-Term Trends in Motor Vehicle Emissions in U.S. Urban Areas, *Environ. Sci. Technol.*, 2013, **47**, 10022–10031.

7 B. C. McDonald, A. H. Goldstein and R. A. Harley, Long-Term Trends in California Mobile Source Emissions and Ambient Concentrations of Black Carbon and Organic Aerosol, *Environ. Sci. Technol.*, 2015, **49**, 5178–5188.

8 K. M. Seltzer, B. N. Murphy, E. A. Pennington, C. Allen, K. Talgo and H. O. T. Pye, Volatile Chemical Product Enhancements to Criteria Pollutants in the United States, *Environ. Sci. Technol.*, 2022, **56**, 6905–6913.

9 X. Tang, P. K. Misztal, W. W. Nazaroff and A. H. Goldstein, Siloxanes Are the Most Abundant Volatile Organic Compound Emitted from Engineering Students in a Classroom, *Environ. Sci. Technol. Lett.*, 2015, **2**, 303–307.

10 B. Molinier, C. Arata, E. F. Katz, D. M. Lunderberg, Y. Liu, P. K. Misztal, W. W. Nazaroff and A. H. Goldstein, Volatile Methyl Siloxanes and Other Organosilicon Compounds in Residential Air, *Environ. Sci. Technol.*, 2022, **56**, 15427–15436.

11 S. M. Charan, Y. Huang, R. S. Buenconsejo, Q. Li, D. R. Cocker Iii and J. H. Seinfeld, Secondary organic aerosol formation from the oxidation of

This journal is © The Royal Society of Chemistry 2025

Environ. Sci.: Processes Impacts, 2025, **27**, 1266–1276 | 1273

decamethylcyclopentasiloxane at atmospherically relevant OH concentrations, *Atmos. Chem. Phys.*, 2022, **22**, 917–928.

12 N. J. Janechek, K. M. Hansen and C. O. Stanier, Comprehensive atmospheric modeling of reactive cyclic siloxanes and their oxidation products, *Atmos. Chem. Phys.*, 2017, **17**, 8357–8370.

13 H. G. Kang, Y. Chen, Y. Park, T. Berkemeier and H. Kim, Volatile oxidation products and secondary organosiloxane aerosol from D5 + OH at varying OH exposures, *Atmos. Chem. Phys.*, 2023, **23**, 14307–14323.

14 M. W. Alton and E. C. Browne, Atmospheric Degradation of Cyclic Volatile Methyl Siloxanes: Radical Chemistry and Oxidation Products, *ACS Environ. Au*, 2022, **2**, 263–274.

15 S. Genualdi, T. Harner, Y. Cheng, M. MacLeod, K. M. Hansen, R. van Egmond, M. Shoeib and S. C. Lee, Global Distribution of Linear and Cyclic Volatile Methyl Siloxanes in Air, *Environ. Sci. Technol.*, 2011, **45**, 3349–3354.

16 R. Xiao, I. Zammit, Z. Wei, W.-P. Hu, M. MacLeod and R. Spinney, Kinetics and Mechanism of the Oxidation of Cyclic Methylsiloxanes by Hydroxyl Radical in the Gas Phase: An Experimental and Theoretical Study, *Environ. Sci. Technol.*, 2015, **49**, 13322–13330.

17 C. Balducci, M. Perilli, P. Romagnoli and A. Cecinato, New developments on emerging organic pollutants in the atmosphere, *Environ. Sci. Pollut. Res.*, 2012, **19**, 1875–1884.

18 D. Brooke, M. Crookes, D. Gray and S. Robertson, *Environmental Risk Assessment Report: Decamethylcyclopentasiloxane*, Environment Agency of England and Wales, Bristol, UK, 2009.

19 C. Rücker and K. Kümmerer, Environmental Chemistry of Organosiloxanes, *Chem. Rev.*, 2015, **115**, 466–524.

20 D.-G. Wang, W. Norwood, M. Alaee, J. D. Byer and S. Brimble, Review of recent advances in research on the toxicity, detection, occurrence and fate of cyclic volatile methyl siloxanes in the environment, *Chemosphere*, 2013, **93**, 711–725.

21 N. A. Warner, A. Evenset, G. Christensen, G. W. Gabrielsen, K. Borgå and H. Leknes, Volatile Siloxanes in the European Arctic: Assessment of Sources and Spatial Distribution, *Environ. Sci. Technol.*, 2010, **44**, 7705–7710.

22 U. E. Agency, *Registry of Restrictions*, 2024.

23 R. Yucuis, C. Stanier and K. Hornbuckle, Cyclic siloxanes in air, including identification of high levels in Chicago and distinct diurnal variation, *Chemosphere*, 2013, **92**, 905–910.

24 A. M. Buser, A. Kierkegaard, C. Bogdal, M. MacLeod, M. Scheringer and K. Hungerbühler, Concentrations in Ambient Air and Emissions of Cyclic Volatile Methylsiloxanes in Zurich, Switzerland, *Environ. Sci. Technol.*, 2013, **47**, 7045–7051.

25 E. Gallego, J. F. Perales, F. J. Roca, X. Guardino and E. Gadea, Volatile methyl siloxanes (VMS) concentrations in outdoor air of several Catalan urban areas, *Atmos. Environ.*, 2017, **155**, 108–118.

26 L. Ahrens, T. Harner and M. Shoeib, Temporal Variations of Cyclic and Linear Volatile Methylsiloxanes in the Atmosphere Using Passive Samplers and High-Volume Air Samplers, *Environ. Sci. Technol.*, 2014, **48**, 9374–9381.

27 A. Kierkegaard and M. S. McLachlan, Determination of decamethylcyclopentasiloxane in air using commercial solid phase extraction cartridges, *J. Chromatogr. A*, 2010, **1217**, 3557–3560.

28 T. Yang, J. Xiong, X. Tang and P. K. Misztal, Predicting Indoor Emissions of Cyclic Volatile Methylsiloxanes from the Use of Personal Care Products by University Students, *Environ. Sci. Technol.*, 2018, **52**, 14208–14215.

29 D. Mackay, C. E. Cowan-Ellsberry, D. E. Powell, K. B. Woodburn, S. Xu, G. E. Kozerski and J. Kim, Decamethylcyclopentasiloxane (D5) environmental sources, fate, transport, and routes of exposure, *Environ. Toxicol. Chem.*, 2015, **34**, 2689–2702.

30 T. M. Tran, K. O. Abualnaja, A. G. Asimakopoulos, A. Covaci, B. Gevao, B. Johnson-Restrepo, T. A. Kumosani, G. Malarvannan, T. B. Minh, H.-B. Moon, H. Nakata, R. K. Sinha and K. Kannan, A survey of cyclic and linear siloxanes in indoor dust and their implications for human exposures in twelve countries, *Environ. Int.*, 2015, **78**, 39–44.

31 A. M. Buser, C. Bogdal, M. MacLeod and M. Scheringer, Emissions of decamethylcyclopentasiloxane from Chicago, *Chemosphere*, 2014, **107**, 473–475.

32 M. M. Coggon, B. C. McDonald, A. Vlasenko, P. R. Veres, F. Bernard, A. R. Koss, B. Yuan, J. B. Gilman, J. Peischl, K. C. Aikin, J. DuRant, C. Warneke, S.-M. Li and J. A. de Gouw, Diurnal Variability and Emission Pattern of Decamethylcyclopentasiloxane (D5) from the Application of Personal Care Products in Two North American Cities, *Environ. Sci. Technol.*, 2018, **52**, 5610–5618.

33 T. B. Low and D. R. Hudak, Development of air mass climatology analysis for the determination of characteristic marine atmospheres. Part I: North Atlantic, *Theor. Appl. Climatol.*, 1997, **57**, 135–153.

34 R. V. Rohli, C. Li, R. V. Rohli and C. Li, *Air Masses*, Meteorology for Coastal Scientists, 2021, pp. 213–218.

35 U. S. C. Bureau, 2020 *U.S. Census Population Density Map*, (accessed 08/08, 2024).

36 NOaA Administration, *U.S. Climate Normals*, 2023, p. 2024.

37 P. Wolkoff, Impact of air velocity, temperature, humidity, and air on long-term voc emissions from building products, *Atmos. Environ.*, 1998, **32**, 2659–2668.

38 R. Wexler, Theory and observations of land and sea breezes, *Bull. Am. Meteorol. Soc.*, 1946, **27**, 272–287.

39 K. Bouchlaghem, F. B. Mansour and S. Elouragini, Impact of a sea breeze event on air pollution at the Eastern Tunisian Coast, *Atmos. Res.*, 2007, **86**, 162–172.

40 B. Yuan, A. R. Koss, C. Warneke, M. Coggon, K. Sekimoto and J. A. de Gouw, Proton-Transfer-Reaction Mass Spectrometry: Applications in Atmospheric Sciences, *Chem. Rev.*, 2017, **117**, 13187–13229.

41 H. Li, M. Riva, P. Rantala, L. Heikkinen, K. Daellenbach, J. E. Krechmer, P. M. Flaud, D. Worsnop, M. Kulmala, E. Villenave, E. Perraudin, M. Ehn and F. Bianchi,

1274 | *Environ. Sci.: Processes Impacts*, 2025, **27**, 1266–1276

This journal is © The Royal Society of Chemistry 2025

Terpenes and their oxidation products in the French Landes forest: insights from Vocus PTR-TOF measurements, *Atmos. Chem. Phys.*, 2020, **20**, 1941–1959.

42 Y. Zhu, S. Guo and W. Liang, A literature review investigating the impact of temperature and humidity on volatile organic compound emissions from building materials, *Build. Environ.*, 2024, **262**, 111845.

43 J. Krechmer, F. Lopez-Hilfiker, A. Koss, M. Hutterli, C. Stoermer, B. Deming, J. Kimmel, C. Warneke, R. Holzinger, J. Jayne, D. Worsnop, K. Fuhrer, M. Gonin and J. de Gouw, Evaluation of a New Reagent-Ion Source and Focusing Ion-Molecule Reactor for Use in Proton-Transfer-Reaction Mass Spectrometry, *Anal. Chem.*, 2018, **90**, 12011–12018.

44 T. Bruderer, M. T. Gaugg, L. Cappellin, F. Lopez-Hilfiker, M. Hutterli, N. Perkins, R. Zenobi and A. Moeller, Detection of Volatile Organic Compounds with Secondary Electrospray Ionization and Proton Transfer Reaction High-Resolution Mass Spectrometry: A Feature Comparison, *J. Am. Soc. Mass Spectrom.*, 2020, **31**, 1632–1640.

45 C. Rivera, J. Mellqvist, J. Samuelsson, B. Lefer, S. Alvarez and M. R. Patel, Quantification of NO2 and SO2 emissions from the Houston Ship Channel and Texas City industrial areas during the 2006 Texas Air Quality Study, *J. Geophys. Res.:Atmos.*, 2010, **115**, D08301.

46 G. Earth, *Map of Cane Island, TX*, Map of a House in Cane Island, TX, 2023.

47 U.S. Census Bureau, *Number of Households in the U.S. from 1960 to 2023 (in millions)*, https://www.census.gov/data/tables/time-series/demo/families/households.html, accessed 2024, August.

48 R. E. School, *Robertson Elementary 2023-2024 Campus Improvement Plan*, 2023.

49 J. Seinfeld, *Atmospheric Physics and Chemistry of Air Pollution*, 1985.

50 R. Atkinson, Kinetics of the gas-phase reactions of a series of organosilicon compounds with hydroxyl and nitrate(NO3) radicals and ozone at 297 +− 2 K, *Environ. Sci. Technol.*, 1991, **25**, 863–866.

51 US EPA Office of Research and Development, *CMAQ (5.0.1)*, 2012, DOI: 10.5281/zenodo.13883210.

52 J. G. Powers, J. B. Klemp, W. C. Skamarock, C. A. Davis, J. Dudhia, D. O. Gill, J. L. Coen, D. J. Gochis, R. Ahmadov, S. E. Peckham, G. A. Grell, J. Michalakes, S. Trahan, S. G. Benjamin, C. R. Alexander, G. J. Dimego, W. Wang, C. S. Schwartz, G. S. Romine, Z. Liu, C. Snyder, F. Chen, M. J. Barlage, W. Yu and M. G. Duda, The Weather Research and Forecasting Model: Overview, System Efforts, and Future Directions, *Bull. Am. Meteorol. Soc.*, 2017, **98**, 1717–1737.

53 H. Hersbach, B. Bell, P. Berrisford, S. Hirahara, A. Horányi, J. Muñoz-Sabater, J. Nicolas, C. Peubey, R. Radu, D. Schepers, A. Simmons, C. Soci, S. Abdalla, X. Abellan, G. Balsamo, P. Bechtold, G. Biavati, J. Bidlot, M. Bonavita, G. De Chiara, P. Dahlgren, D. Dee, M. Diamantakis, R. Dragani, J. Flemming, R. Forbes, M. Fuentes, A. Geer, L. Haimberger, S. Healy, R. J. Hogan, E. Hólm, M. Janisková, S. Keeley, P. Laloyaux, P. Lopez, C. Lupu, G. Radnoti, P. de Rosnay, I. Rozum, F. Vamborg, S. Villaume and J.-N. Thépaut, The ERA5 global reanalysis, *Q. J. R. Meteorol. Soc.*, 2020, **146**, 1999–2049.

54 D. Van Hoomissen, A. Chattopadhyay and J. B. Burkholder, Rate Coefficients for the Cl Atom Gas-Phase Reaction With Permethylsiloxanes (PMS): L2, L3, L4, L5, D3, D4, D5, and D6, *Int. J. Chem. Kinet.*, 2025, **57**, 213–231.

55 H. Stark, R. L. N. Yatavelli, S. L. Thompson, J. R. Kimmel, M. J. Cubison, P. S. Chhabra, M. R. Canagaratna, J. T. Jayne, D. R. Worsnop and J. L. Jimenez, Methods to extract molecular and bulk chemical information from series of complex mass spectra with limited mass resolution, *Int. J. Mass Spectrom.*, 2015, **389**, 26–38.

56 C. Yan, W. Nie, M. Äijälä, M. P. Rissanen, M. R. Canagaratna, P. Massoli, H. Junninen, T. Jokinen, N. Sarnela, S. A. K. Häme, S. Schobesberger, F. Canonaco, L. Yao, A. S. H. Prévôt, T. Petäjä, M. Kulmala, M. Sipilä, D. R. Worsnop and M. Ehn, Source characterization of highly oxidized multifunctional compounds in a boreal forest environment using positive matrix factorization, *Atmos. Chem. Phys.*, 2016, **16**, 12715–12731.

57 H. Schnadt and I. Ivanov, in *Nuclear Safety in Light Water Reactors*, ed. B. R. Sehgal, Academic Press, Boston, 2012, doi: DOI: 10.1016/B978-0-12-388446-6.00007-1, pp. 589–624.

58 V. Yavuz, Unveiling the impact of temperature inversions on air quality: a comprehensive analysis of polluted and severe polluted days in Istanbul, *Acta Geophys.*, 2024, **73**, 969–986.

59 D. C. Dowell, C. R. Alexander, E. P. James, S. S. Weygandt, S. G. Benjamin, G. S. Manikin, B. T. Blake, J. M. Brown, J. B. Olson, M. Hu, T. G. Smirnova, T. Ladwig, J. S. Kenyon, R. Ahmadov, D. D. Turner, J. D. Duda and T. I. Alcott, The High-Resolution Rapid Refresh (HRRR): An Hourly Updating Convection-Allowing Forecast Model. Part I: Motivation and System Description, *Weather Forecast.*, 2022, **37**, 1371–1395.

60 W. G. Blumberg, K. T. Halbert, T. A. Supinie, P. T. Marsh, R. L. Thompson and J. A. Hart, SHARPpy: An Open-Source Sounding Analysis Toolkit for the Atmospheric Sciences, *Bull. Am. Meteorol. Soc.*, 2017, **98**, 1625–1636.

61 C. R. Harris, K. J. Millman, S. J. van der Walt, R. Gommers, P. Virtanen, D. Cournapeau, E. Wieser, J. Taylor, S. Berg, N. J. Smith, R. Kern, M. Picus, S. Hoyer, M. H. van Kerkwijk, M. Brett, A. Haldane, J. F. del Río, M. Wiebe, P. Peterson, P. Gérard-Marchant, K. Sheppard, T. Reddy, W. Weckesser, H. Abbasi, C. Gohlke and T. E. Oliphant, Array programming with NumPy, *Nature*, 2020, **585**, 357–362.

62 J. D. Hunter, Matplotlib: A 2D Graphics Environment, *Comput. Sci. Eng.*, 2007, **9**, 90–95.

63 Tpd team, *pandas*, 2024, 1.3.2.

64 S. Hoyer and J. Hamman, xarray: N-D labeled Arrays and Datasets in Python, *J. Open Res. Softw*, 2017, **5**(1), 10.

This journal is © The Royal Society of Chemistry 2025

Environ. Sci.: Processes Impacts, 2025, **27**, 1266–1276 | 1275

65 T. Dudzina, E. Garcia Hidalgo, N. von Goetz, C. Bogdal and K. Hungerbuehler, Evaporation of decamethylcyclopentasiloxane (D5) from selected cosmetic products: Implications for consumer exposure modeling, *Environ. Int.*, 2015, **84**, 55–63.

66 C. E. Brunet, R. F. Marek, C. O. Stanier and K. C. Hornbuckle, Concentrations of Volatile Methyl Siloxanes in New York City Reflect Emissions from Personal Care and Industrial Use, *Environ. Sci. Technol.*, 2024, **58**, 8835–8845.

67 *How often do you use antiperspirant or deodorant?*, https://today.yougov.com/topics/society/survey-results/daily/2024/07/02/1664c/3, accessed March, 2025.

68 T. L. Yuxuan Wan, G. Roberts, S. Wasti and X. Liu, *Final Report For Grant Activities No. 582-23-43887-030 Ozone-NOx-VOC Sensitivity In Texas Urban Areas Category III, Research Model Development Or Application Texas Comission on Environmental Quality*, Texas Comission on Environmental Quality, 2024.

69 J. G. Navea, M. A. Young, S. Xu, V. H. Grassian and C. O. Stanier, The atmospheric lifetimes and concentrations of cyclic methylsiloxanes octamethylcyclotetrasiloxane (D4) and decamethylcyclopentasiloxane (D5) and the influence of heterogeneous uptake, *Atmos. Environ.*, 2011, **45**, 3181–3191.

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