Optimization and Representativeness of Atmospheric Chemical Sampling by Hovering Unmanned Aerial Vehicles Over Tropical Forests

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Abstract Atmospheric chemical species play critical roles in ecosystem functioning and climate, but spatially resolving near-surface concentrations has been challenging. In this regard, hovering unmanned aerial vehicles (UAVs) represent an emerging technology. The study herein provides guidance for optimized atmospheric sampling by hovering copter-type UAVs. Large-eddy simulations are conducted for species having chemical lifetimes ranging from reactive (i.e., $10^2$ s) to long-lived (i.e., $10^8$ s). The case study of fair-weather conditions over an equatorial tropical forest is used because of previous UAV deployments in this region. A framework is developed of influence length and horizontal shift of upwind surface emissions. The framework quantifies the length scale of the contribution of upwind forest emissions to species concentrations sampled by the downwind hovering UAV. Main findings include the following: (1) sampling within an altitude that is no more than 200 m above the canopy is recommended for both high- and intermediate-reactivity species because of the strong decrease in species concentration even in a highly turbulent atmosphere; (2) sampling durations of at least 5 and 10 min are recommended for intermediate- and high-reactivity species, respectively, because of the effects of atmospheric turbulence; and (3) in the case of heterogeneity of emissions across the underlying landscape, maximum recommended altitudes are presented for horizontal sampling strategies that can resolve the variability in the landscape emissions. The coupled effects of emission rate, wind speed, species lifetime, turbulence, and UAV sampling duration on influence length must all be considered for optimized and representative sampling over forests.

1. Introduction

Plant landscapes serve as huge reservoirs of organic and inorganic chemical species that dynamically exchange between the biosphere and the atmosphere (Ashworth et al., 2015; Costa, 2011; Faiola et al., 2018; Li et al., 2016; Malmheimer et al., 2011; Pandey et al., 2019). In recent years, sampling and process studies of atmospheric species concentrations over landscapes have used available platforms such as tethered balloons, aircraft, satellites, and towers, each of which offers excellent measurements at certain scales (Table 1). Tethered balloons can provide excellent vertical resolution for sampling, although they are often difficult to control and offer limited capability for horizontal sampling strategies (Tompkins, 2002). Aircraft data sets provide a unique atmospheric perspective, typically for altitudes of 500 m and higher (Ajaj et al., 2016; Krabill et al., 2002; Y. Liu et al., 2018). Sampling below these altitudes near the surface with aircraft is often not possible for technical and regulatory reasons. Given the speed and altitude of aircraft, depending on the scale of forest heterogeneity the collected data sets typically represent the average of emission rates across several landscape sub-types and face challenges in data inversion for resolving any near-surface gradients in species concentrations (Bela et al., 2015; Krejci et al., 2003; Lelievel et al., 2008; Martin et al., 2016). Satellite platforms have the advantage of frequent global coverage, yet the horizontal...
resolution is typically limited to several kilometers and affected by cloud cover (Duncan et al., 2010). Furthermore, the vertical resolution of a species concentration near the surface approaches the entire height of the planetary boundary layer for many species. Data inversion from columnar observations by satellite instrumentation to in-situ near-surface concentrations can have large uncertainties (Millet et al., 2006; Peng et al., 2015; Potter et al., 2001).

The most numerous and extensive data sets for many atmospheric species are based on measurements from towers. Towers are usually constructed on plateau regions of the forest to guarantee a foundation built on well-drained and strong soils (Avissar et al., 2002). The tower height typically extends 10–20 m above the forest canopy, although some towers can approach 300 m in height (Andreae et al., 2015). These towers provide excellent accessibility for monitoring the near-surface concentrations of atmospheric species in a continuous time series (Martin et al., 2010; Nölscher et al., 2016; Williams et al., 2016; Yáñez-Serrano et al., 2015). In some cases, however, depending on the species chemical lifetime and the characteristic times of species advection and convection, near-surface species concentrations can be horizontally heterogeneous across the landscape. For these species, the data sets from a tower might represent the emissions of the nearby forest surrounding the tower but might have negative or positive bias when extrapolated to other locations of the forest. For instance, a study in the central Amazon found that isoprene concentrations were consistently higher by an average of 60% over a plateau forest compared to a nearby slope forest (Batista et al., 2019). The separation distance between the two forest sub-types was 700 m.

In the context of the capabilities and limitations of each of these different measurement platforms, copter-type hovering unmanned aerial vehicles (UAVs) of 25 kg or less are emerging as a cost-effective and capable platform to complement and supplement other sampling platforms (Table 1) (Stewart & Martin, 2020a). The upper limit of a hovering UAV take-off mass of 25 kg is set for most scientists by the regulatory licensing requirements of many countries, and heavier take-off mass often requires considerable additional professional licensing and training (Stewart & Martin, 2020b). Hovering UAVs of 25 kg and lighter are especially promising for filling data gaps in near-surface concentrations for species that are horizontally heterogeneous above the landscape on scales of 10–1,000 m (Chang et al., 2018; McKinney et al., 2019). Atmospheric measurements can be achieved by mounting compact sensors or samplers onto UAVs of 1–25 kg (Aurell et al., 2017; Black et al., 2018; Guimarães et al., 2019, 2020; B. Liu et al., 2020; McKinney et al., 2019; Neumann et al., 2019; Ye et al., 2020). For example, Aurell et al. (2017) installed an emission sampler system on a hovering UAV to characterize the gas and particle emissions from open fires and thereby followed the transport of the combustion plume. Using a hovering UAV equipped with absorbent samples and subsequent off-line analyses, Black et al. (2018) measured atmospheric gaseous mercury concentrations and demonstrated the maneuverability of the UAV as an advantage for source characterization. Neumann et al. (2019) installed a lightweight laser-based gas sensor on a UAV for detection of surface methane leaks. New sensors suitable for mid-range UAV platforms are an active area of research and development, and important developments of new capabilities can be expected in the coming years (Stewart & Martin, 2020a). For instrumentation that is too heavy for the UAV, the UAV can instead elevate a long sampling tube (e.g.,

| Table 1 |
| --- |
| Comparison of Atmospheric Platforms Used to Identify and Measure the Concentrations of Chemical Species |
| Horizontal resolution – Tower 10's–100's of m | Copter-type hovering UAV 1's–10's of m | Fixed-wing UAV 10's–100's of m | Aircraft 1's–10's of km | Satellite 1's–10's of km |
| Vertical resolution 1's m | 1's–10's of m | 1's–10's of km | 10's–100's of m | BL |
| Vertical height Ground to tower height | Ground to BL top | Ground to BL top | 10's of m to BL top | 500 m to BL top | – |
| Operation feasibility Easy | Difficult | Easy–medium | Easy–medium | Difficult | Difficult–very difficult |
| Measurement cost $$ | $$ | $ | $$ | $$$–$$$$ |

Note. The effective spatial resolution for UAV and aircraft measurements takes into consideration the flight speed and the typical times required for analytical sampling.

Abbreviations: BL, boundary layer; UAV, unmanned aerial vehicle.

*aSubject to UAV aviation policy and regulations.*
>100 m) that is connected to analytical instrumentation at the ground level for real-time measurement (Shah et al., 2019). A drawback of this approach is that sticky or reactive chemical species can be lost to the tubing walls. Studies to date demonstrate the capabilities of hovering UAVs as platforms for measurements of species concentrations at vertical and horizontal resolutions of 1–10 m and time resolutions of seconds to minutes (Table 1).

For this newly emerging measurement platform of hovering UAVs, practical guidelines for scientifically meaningful sampling, such as sampling height and sampling duration to achieve specific scientific goals, are in need of development. Among studies to date that have deployed hovering UAVs, chemical lifetimes of the target species, the sampling location of the UAV, and the microscale meteorology (e.g., atmospheric thermodynamic conditions and winds) have varied from study to study without detailed attention to optimization strategies for the specific goals of the different studies. Herein, in a systematic fashion, a state-of-the-art model, the Dutch Atmospheric Large-Eddy Simulation (DALES) coupled with an online chemical module, is utilized to investigate the role of atmospheric transport, in conjunction with chemical variables and microscale meteorology, for sampling strategies by hovering UAVs near the Earth's surface at horizontal scales of a few hundred meters. The focus of the simulations is on the application and optimization of sampling strategies for hovering copter-type UAVs over landscapes of homogeneous compared to heterogeneous emission rates. Key questions that are addressed include: (i) how long must a hovering UAV collect a sample to obtain a representativeness that is independent of local turbulence and (ii) what is the relation between UAV sampling altitude and the possibility for spatial resolution of heterogeneity in landscape emissions.

The boundary layer over the Amazon forest under fair-weather conditions and the emissions and lifetime of volatile organic compounds (VOCs) from the forest are selected as an example for the study herein by DALES for several reasons. Volatile organic compounds play pivotal roles in ecosystem functioning for signaling among plants, animals, and microbes and as reactants in atmospheric chemistry (Jardine & Jardine, 2016; Seco et al., 2015). The concentrations and types of VOCs over tropical forests vary enormously horizontally in response to the underlying heterogeneity in the vegetation. The emission rates of different VOCs are affected by factors such as rainfall, sunlight, temperature, soil fertility, disease, and pestilence, among others. VOC species have a wide range of reactive-loss chemical lifetimes in the atmosphere and thus provide a fertile framework for study in the DALES framework. In earlier work by the authors, an observational program by UAVs took place in the central Amazon, and the data set implied a landscape of heterogeneous VOC emissions (Batista et al., 2019). The VOC sampler was pre-programmed and mounted to the UAV for autonomous sampling (McKinney et al., 2019). Real-time communication was maintained between the handheld user interface and the sampler and the UAV during flight. The DALES product was previously applied and validated for the central Amazon (Ouwersloot et al., 2011; Vilà-Guerau de Arellano et al., 2011). A thorough evaluation and intercomparison among the DALES simulation results, field observations, and a mesoscale weather forecast model is presented in Vilà-Guerau de Arellano et al. (2019) for the central Amazon.

### 2. Numerical Methodology

Atmospheric turbulent transport is simulated by DALES (Version 4.1) (Heus et al., 2010). The filtered Navier-Stokes equations under the Boussinesq approximation is used to resolve eddies larger than the filter scale (i.e., the simulation resolution). A one-and-a-half-order closure is applied to parameterize the sub-filter-scale processes. A periodic boundary condition is employed in the horizontal direction. An on-line chemical module within DALES couples boundary layer dynamics and atmospheric chemical processes (Vilà-Guerau de Arellano et al., 2005). The experimental parameters used in the reference simulation and varied across the set of sensitivity analyses of this study are listed in Table S1.

For the numerical experiments described herein, simulations are carried out for 3 h. The resolutions in the direction of parallel winds, cross winds, and altitude are 20 × 20 × 20 m, respectively, across a grid of 2560 × 160 × 128 equally spaced points. This domain size is large enough to obviate an influence by the periodic boundary condition. The DALES filter width of 20 m is sufficient to resolve more than 90% of the turbulent energy (Heus et al., 2010). The grid resolution of the simulation (i.e., 20 m) is significantly greater than the disturbance scale induced by the rotors of common commercially available UAVs (Haas...
et al., 2014; Lampert et al., 2020; Ventura Diaz & Yoon, 2018), and as such the simulation results are not significantly affected by rotor disturbance (see Section 4.3). A simulation time step of 1 s is used to avoid instability of the chemical solver (Ouwersloot et al., 2011). The numerical uncertainty of DALES is presented in Section S1 of the Supplementary Information (Figure S1).

The presented results focus on noontime when the turbulent boundary layer is strongly developed. Meteorological and chemical data representative of a typical cloud-free day in the central Amazon are used for the boundary conditions (Batista et al., 2019; Ouwersloot et al., 2011). A wind speed of 2 m s⁻¹ at 50 m, meaning 20 m above canopy, holds unless otherwise stated. A logarithmic wind profile, described by $u_k = (u^* / \kappa_V) \ln \left( \frac{(z_k - d)}{z_0} \right)$, is used to initiate the model. Parameters include a friction velocity $u^*$ of 0.25 m s⁻¹, a Von Kármán constant $\kappa_V$ of 0.4, a displacement height $d$ of 75% of the canopy height, and a roughness length $z_0$ of 0.10 m (Batista et al., 2019; Ouwersloot et al., 2011). A longer roughness length of 1.0 m was also tested without significant changes to the quantitative conclusions of this study. Solar radiation corresponds to a clear sky on February 28, 2018 at the Adolfo Ducke Forest Reserve (3.003°S, 59.940°W), Manaus, Brazil. This location and time are chosen because UAV flights took place at the reserve at that time (Batista et al., 2019). Other parameter settings for the simulations are adapted from Ouwersloot et al. (2011) (Section S2). That study also performed DALES simulations for the central Amazon, though unrelated to UAV sampling. For the parameters used in this study, the timescale for convection in the daytime boundary layer, represented by the largest eddies, is <10³ s (Section S3).

For chemical reactions, the analyses herein focus on a case study of the reactive loss of VOCs by oxidation with hydroxyl radical (OH) and ozone (O₃). Chemical reactions of different VOC species $i$, labeled as VOC$_i$, are expressed as follows:

$$\text{VOC}_i + \text{OH and/or O}_3 \rightarrow \text{products}$$

The reaction rate $R_i$ of species $i$ is calculated as follows:

$$R_i = -\left( k_{\text{OH},i} [\text{OH}] + k_{\text{O}_3,i} [\text{O}_3] \right) [\text{VOC}_i] = -k_i [\text{VOC}_i] = -[\text{VOC}_i] / \tau_i$$

where $k_{\text{OH},i}$ and $k_{\text{O}_3,i}$ are the bimolecular rate constants of VOC/OH and VOC/O₃ reactions, respectively; $[\text{OH}]$, $[\text{O}_3]$, and $[\text{VOC}_i]$ are the concentrations of hydroxyl radical, ozone, and VOC species $i$, respectively; $k_i$ is the pseudo first-order reaction rate constant given by $(k_{\text{OH},i} [\text{OH}] + k_{\text{O}_3,i} [\text{O}_3])$; $\tau_i$ is the chemical lifetime of VOC given by $1/k_i$; and the negative sign of Equation 2 indicates reactive loss (i.e., negative reaction rate). For simplicity, oxidant concentrations (i.e., $[\text{OH}]$ and $[\text{O}_3]$) are fixed within the simulation domain. Specific values of $k_{\text{OH},i}$, $k_i$, $[\text{OH}]$, and $[\text{O}_3]$ are not stated in this study because in product they correspond to a single parameter $\tau_i$ within Equation 2. Chemical compounds having lifetimes of 10² s (e.g., for sesquiterpenes [Rantala, 2016]) to 10⁸ s (e.g., for methane [Hopcroft et al., 2017]) are investigated across the set of numerical experiments.

3. Results and Discussion

3.1. Sampling Over a Landscape of Homogeneous Emission Rates

Simulations were performed to investigate the concentration distributions of different species in the atmospheric boundary layer over a land surface characterized by homogeneous emission rates.

3.1.1. Vertical Variability of VOC Concentrations (Homogeneous Emissions)

Figure 1 shows the concentrations for species having chemical lifetimes of 10², 10⁵, and 10⁸ s, representing VOC species of high, intermediate, and low reactivity, respectively. For high-reactivity compounds (i.e., short lifetimes), such as the VOC group of sesquiterpenes, concentrations decrease sharply in the lower part of the boundary layer because of rapid atmospheric chemical reactions (Figures 1a and 1d). For low-reactivity species, such as the VOC methane (i.e., long lifetime), the concentrations change little with height. The concentration depends on the local emission rate of the VOC as well as its regional background concentration (Figures 1c and 1f). By comparison to the simple concentration profiles of the two limiting extremes of high- and low-reactivity species, concentrations for intermediate-reactivity species are more complex.
Example species include oxygenated VOCs like ethanol, formaldehyde, and methyl vinyl ketone. The concentrations decrease in the roughness layer, hold steady in the boundary layer, and drop in the free troposphere. The roughness layer constitutes approximately three canopy heights. Above this layer, the concentrations remain approximately constant for several hundred meters. Near the top of the boundary layer, the concentrations drop because of overhead entrainment of VOC-poor air.

The simulated vertical profiles omit dry deposition of the species to the landscape. For VOCs, dry deposition can include passive deposition to surfaces or active stomatal uptake by the vegetation, and as a result dry deposition is highly variable among different VOCs (Matsui et al., 2016). For this reason, dry deposition is omitted in the study. For species that undergo significant dry deposition, however, the profiles shown in Figure 1 can change. Concentrations within the roughness layer compared to above it could be higher (i.e., \( \text{emission} > \text{deposition} \)), equal (i.e., \( \text{emission} = \text{deposition} \)), or lower (i.e., \( \text{emission} < \text{deposition} \)), such as for VOC species like peroxyacetyl nitrate and isoprene hydroxy nitrates that are produced in the atmosphere). Unlike the parameter for dry deposition, changes in other parameters in the simulation, such as wind speed and surface heat flux across typical values, do not significantly impact the shape of the vertical profiles.

### 3.1.2. Horizontal Variability of VOC Concentrations (Homogeneous Emissions)

Figures 1a–1c show that the horizontal variability of VOC concentration is low. It does not depend strongly on species reactivity. This result can be expected for a landscape of homogeneous emissions. Even so, depending on the averaging time, the DALES simulation captures small variations associated with atmospheric turbulent mixing. The horizontal concentration distributions in the near-surface layer for averaging times of 1, 10, and 60 min are presented in Figure S2. These averaging times represent different sampling durations for an analyte by a hovering UAV. The horizontal concentration distributions at different altitudes (i.e., 100, 500, and 1,000 m) are shown in Figure S3 for 1-min averaging.
The variability in the time-averaged concentration, corresponding to multiple sampling of the statistical population of species concentrations associated with turbulence, increases for shorter sampling durations (Figures S2). For sampling at a single point by a single UAV, the variability in simulated concentrations in the near-surface layer is <5% (one-sigma variation) for both high-reactivity species and intermediate-reactivity species for 60-min averaging (Figure S2). By comparison, the variability at a single point increases to 18% and 17% for 1-min averaging of high- and intermediate-reactivity species, respectively. Furthermore, the variability extends from the near-surface layer to the top of the boundary layer (Figure S3). For intermediate-reactivity species, the horizontal variability is 22% and 19% at altitudes of 100 and 1,000 m, respectively, for 1-min averaging (Figure S3). The implication is that the concentration for a single 1-min sample collected by a UAV at those points can vary by about 20% (one-sigma variation) simply because of atmospheric turbulence, without regard to emission rates from the forest or chemical reactions in the atmosphere.

For simultaneous sampling at two or more points by several different UAVs, the statistical population of the ratios $R$ of the near-surface concentrations of a species between any two locations that are 1,000 m apart from each other can be calculated as a function of sampling duration. The separation of 1,000 m is taken as an example to represent the scales of two nearby forest sub-types in the central Amazon (e.g., plateau, slope, or valley forests [Batista et al., 2019]). Significant variability in the ratio from unity can indicate insufficient sampling duration within a turbulent atmosphere. This variability, captured in a calculation of variance, ultimately represents uncertainty in any comparison of concentrations between spatiotemporal points in the atmosphere.

The probability density functions of $R$ for species of high and intermediate reactivity are plotted in Figure 2 for continuous as well as non-consecutive sampling strategies. For continuous sampling, five durations ranging from 5 to 60 min (specifically, 5, 10, 20, 30, and 60 min, in the third hour of the simulation) are considered in the analysis. For non-consecutive sampling, sampling for any four discontinuous 5-min durations in the third hour (i.e., 5 min × 4 = 20 min) is considered. As seen in the figure, longer continuous sampling durations significantly reduce the uncertainty associated with atmospheric turbulent mixing in a comparative analysis of measured concentrations between any two points. The standard deviation $\sigma$ of $R$ around unity corresponds to 12.6% uncertainty for comparative sampling of a high-reactivity species during 5 min, which decreases to 6.2%, 3.4%, 2.5%, and 1.6% for continuous sampling durations of 10, 20, 30, and
60 min, respectively. The standard deviation of comparative sampling also decreases with an increasing lifetime of an atmospheric species. There is 7.4% uncertainty for comparative sampling of an intermediate-reactivity species for 5 min, decreasing to 4.0%, 2.0%, 1.6%, and 1.0% for 10-, 20-, 30-, and 60-min durations, respectively. The analyses also show that there are significant differences between continuous compared to nonconsecutive sampling strategies. For nonconsecutive sampling (i.e., 20 min as four 5-min collections), the uncertainties are 5.2% and 3.6% for comparative sampling of high- and intermediate-reactivity species, respectively. These uncertainties are 3.4% and 2.0%, respectively, for continuous sampling for 20 min (Table S2). This greater uncertainty for nonconsecutive sampling arises because continuous sampling successfully averages across large eddies in ways that nonconsecutive sampling does not, even for the same total duration of sampling.

The analysis presented herein focuses on noontime when turbulence in the boundary layer is typically strongest. Weaker turbulence at other times of the day reduces the uncertainties noted herein by decreasing the standard deviation of the sampled atmospheric concentration for all other factors held the same. Stronger turbulence than simulated for the reference simulation herein is also possible under atmospheric conditions. As a sensitivity test, the surface heat flux was increased by 50% to simulate stronger vertical convection and greater turbulence. The results are listed in Table S2, and changes to the uncertainty in a comparative analysis are not large. For example, the increase in the surface heat flux changed the uncertainty from 7.4% to 7.5% for comparative sampling of an intermediate-reactivity species for 5 min.

These results have important implications for planning effective sampling strategies by hovering UAVs. The sampling duration should be long enough not only to meet the analytical requirements of species quantification but also to reduce the statistical influence of atmospheric turbulence on species concentrations. For single-point sampling, this second aspect is a requirement so that the UAV-sampled concentration can be considered representative of the spatiotemporal point in the atmosphere. For multi-point simultaneous sampling by two or more UAVs, this second aspect is a requirement for meaningful comparative analyses. The optimized sampling duration must take into account the minimum time needed for representativeness, yet the duration should not extend much beyond this minimum so that sampling at several different hovering points within a single UAV flight is possible. Unnecessarily long sampling durations also degrade the time resolution of the data set. The optimized sampling duration for intermediate- and high-reactivity compounds is thus the longer of the analytical requirement related to species quantification or the turbulent requirement related to sufficient averaging to obtain a representative concentration. In the case of the turbulent requirement, a possibility is that the optimized duration could be longer than the hovering-time capability of a given UAV, and in such a case a more capable UAV platform should be sought. These considerations related to atmospheric turbulence thus set a minimum suggested sampling duration.

3.2. Sampling Over a Landscape of Heterogenous Emission Rates

An approach of discrete patches was used to investigate how heterogeneity in emission rates across a landscape relate to UAV sampling of a species concentration in the atmosphere over the landscape. The parallel-wind grid of 2560 points described in the methodology section was divided into 256 contiguous patches of 10 grid points each, each patch thereby corresponding to 200 m in length. The emission rates from 255 of the 256 patches were unchanged from the homogeneous case. Across a series of numerical experiments, the emission rate from the first patch was altered stepwise from −80% to +500% relative to the rate of the homogeneous case (Table S1). Both source and receptor models, also known as prognostic and inverse models, are considered in the analysis (Watson et al., 2002).

3.2.1. Source Model

The vertical profiles above patch 1 are plotted in Figure 3 for high- and intermediate-reactivity species. Compared to the case of a homogeneous emission rate across all patches, an increase of +500% in the emission rate from patch 1 for a high-reactivity species leads to an increase of +225% in its near-surface concentration above patch 1. For a decrease in the emission rate by −80%, the near-surface concentration above patch 1 decreases by −42%. Both these concentration differences decrease significantly with altitude. At 100 m above patch 1, the respective concentration differences are +18% and −6%. For intermediate-reactivity species, the differences are smaller. Near-surface concentrations above patch 1 are respectively +64%
and −11% for the considered cases of higher and lower emission rates. Overall, these results show that heterogeneity in the local emission rate can significantly affect the concentration sampled by instrumentation on a hovering UAV or on a tower that is positioned in the lower part of the boundary layer, at least for species of intermediate and high reactivity.

The fractional contribution of emissions from patch 1 to downwind species concentration is plotted in Figure 4. Results are shown as a function of altitude and distance from the source. The emissions plume travels downwind and upward. Panels a to d of Figure 4 plot the results for different heterogeneity scales for patch 1, ranging from 100 to 800 m. Conditions are for the reference case of Table 2, meaning a species lifetime of $10^3$ s. This lifetime, representing a VOC like isoprene, is similar to the timescale of the biggest eddies in the boundary layer. The fractional contribution is calculated by taking the ratio of the concentrations in each grid point between the simulation results from a heterogeneous emission scenario (rows 9 to 12 in Table S1) and a homogeneous emission scenario (row 4 in Table S1).

The maximum fractional contribution from a source patch to atmospheric concentrations is shifted downwind relative to the patch (Figure 4). For instance, at a height of 100 m the fractional contribution of patch 1 directly overhead is 10% whereas 100 m downwind the contribution is 30%. At a certain altitude, the relative contribution of patch 1 drops below 10% for all downwind distances. At this altitude and for an assumed analytical precision of 10% to a species concentration, the UAV sampling strategy is no longer sensitive to the underlying heterogeneous emissions. This height is recognized to as the blending height (Mahrt, 2000). For Figure 4a, representing a surface heterogeneity of 100 m, the blending height is 80 m. At the blending height, the influence of heterogeneity in underlying surface properties on the vertical distribution of a species or physical parameter is no longer distinguishable, and the atmosphere at that altitude is described as horizontally well mixed.

The blending height varies with the scale of landscape heterogeneity, among other factors. For example, as shown in Figure 4e, for a blending height set at 10% precision based on the analytical method, decreasing the scale of emission heterogeneity from 200 to 100 m lowers the blending height from 210 to 80 m. For an increase in the scale of emission heterogeneity from 200 to 400 m, the blending height rises to 700 m. For an 800-m scale of heterogeneity, the blending height reaches to the boundary layer top of 1,400 m. The boundary layer top, serving as a physical cap on blending height, limits its further increase with the increase of the scale of surface heterogeneity. The blending height also depends on the lifetime of a target species in the atmosphere, and the analysis herein is restricted to a lifetime of $10^3$ s (e.g., isoprene).

### 3.2.2. Receptor Model

A receptor model, also known as an inverse model, is used here to investigate the upwind influence on local concentrations (Watson et al., 2002). A zone of influence is defined as an upwind distance across which the landscape emissions affect the concentration of a target species at the point of UAV sampling (Batista...
The zone size depends on the physical properties of the landscape surface, the atmospheric lifetime of the target species, and other environmental parameters. For zone sizes larger than 10's of m, the local disturbance of the atmosphere by the rotors of a UAV that is 25 kg or smaller does not further increase zone size (Crazzolara et al., 2019; Hass et al., 2014; Lampert et al., 2020).

The upwind influence is investigated, as follows. The concentration sampled by a hovering UAV for the case of a homogeneous emission rate across the entire landscape is compared to that sampled for a modified case that has zero emissions across a swath of upwind landscape. The swath of zero emissions starts at the landscape below the hovering UAV, possibly offset by an upwind horizontal shift $\delta$ from the overhead UAV. The swath extends upwind from $\delta$ by a horizontal distance $\lambda_x$ (Figure 5). When the wind speed is faster than the characteristic time of vertical turbulence, an upwind horizontal shift $\delta$ occurs. This shift corresponds to the horizontal distance originating directly below the UAV that contributes to <1% of the concentration sampled by the UAV. A zone of influence of $x\%$ corresponds to the horizontal distance $\lambda_x$ for which an adjustment of the emission rate to zero leads to a decrease of $x\%$ in the species concentration at the point of UAV sampling (Figure S4). Typical choices of $x\%$ in this study are 63% (Figures 5 and 6) as well as 25%, 50%, and 75% (Table 3). Hereafter, when stated as $\lambda$ without further information, the implication is $\lambda_{63\%}$. Both $\lambda$ and $\delta$ increase with sampling height (Figure 5).

Figure 4. Source model showing the fractional contribution of emissions from patch 1 to the total atmospheric concentration. Panels (a) through (d) represent different scales of heterogeneity for patch 1: (a) 100 m, (b) 200 m, (c) 400 m, and (d) 800 m. Panel (e) plots the blending height as a function of the size of surface heterogeneity in emissions. The dashed line represents the planetary boundary layer height (PBLH). Plots are for a species having a chemical lifetime of $10^3$ s.
The numerical experiments further examine the effects of sampling height, wind speed, and chemical life-time on $\lambda$ and $\delta$ (Table 2 and Figure 6). For sampling heights from 50 to 450 m, $\lambda$ increases from 610 to 3,660 m, and $\delta$ increases from 50 to 620 m. For wind speeds of 1–3 m s$^{-1}$, $\lambda$ increases from 350 to 880 m, and $\delta$ increases from 10 to 90 m. For surface heat fluxes of 0.05–0.15 K m s$^{-1}$, $\lambda$ decreases from 720 to 540 m, and $\delta$ decreases from 70 to 50 m (cf. rows 11 to 13, Table 2), which are due to the suppression of vertical convection and turbulence. For chemical lifetimes of $10^2$–$10^5$ s, $\lambda$ increases from 310 to 15,000 m, and $\delta$ increases from 30 to 90 m. The effect of lifetime on $\lambda$ and $\delta$ saturates above $10^5$ s because the influence of transport by advection and convection exceeds that of chemical loss for the distribution of species concentration throughout the boundary layer. For species having a lifetime longer than $10^5$ s, the Damköhler

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### Table 2

| Simulation                      | Input         | Output       |
|--------------------------------|---------------|--------------|
|                                | $\tau$ (s)    | $u$ (m s$^{-1}$) | $H$ (K m s$^{-1}$) | $\lambda$ (m) | $\delta$ (m) |
| 1 Reference                    | $10^3$        | 2.0          | 0.10            | 610           | 50           |
| 2 Horizontal wind speed        | $10^3$        | 1.0          | 0.10            | 350           | 10           |
| 3                              | –             | 1.5          | –               | 450           | 30           |
| 4b                             | –             | 2.0          | –               | 610           | 50           |
| 5                              | –             | 2.5          | –               | 740           | 70           |
| 6                              | –             | 3.0          | –               | 880           | 90           |
| 7 Atmospheric species lifetime | $10^2$        | 2.0          | 0.10            | 310           | 30           |
| 8b                             | $10^3$        | –            | –               | 610           | 50           |
| 9                              | $10^4$        | –            | –               | 11,030        | 80           |
| 10                             | $\geq10^5$    | –            | –               | 15,300        | 90           |
| 11 Surface heat flux           | $10^5$        | 2.0          | 0.05            | 720           | 70           |
| 12b                            | –             | –            | 0.10            | 610           | 50           |
| 13                             | –             | –            | 0.15            | 540           | 50           |

**Notes.** The influence length corresponds to a 63% contribution by the emissions from a swath of underlying landscape (i.e., length) to the concentration sampled by the hovering UAV. Results are listed in the top row for a reference simulation and in the following rows for comparative changes relative to the reference simulation. Varied input quantities in the simulations include horizontal wind speed $u$, atmospheric species lifetime $\tau$, and surface heat flux $H$.

*a*See methodology section for the altitude dependence of wind speed. *b*Identical to reference case in first row.

The receptor model showing the influence length $\lambda$ (dark yellow bar; representing zone of influence of 0%–63%) and horizontal shift $\delta$ (blue bar; representing the zero-influence zone associated with near-field advection) as a function of sampling height. The height of the forest landscape is 30 m. Plot is for a species having a chemical lifetime of $10^5$ s.
number is $\ll 1$ in the turbulent boundary layer (Damköhler, 1940). For these long-lived species, mixing of the boundary layer occurs rapidly relative to chemical reaction rates (Section S4) (Vilà-Guerau de Arellano et al., 2003; 2004).

The results of this DALES study regarding the contribution of emissions from the underlying and upwind landscape to concentrations sampled by the hovering UAV can be compared to those of Batista et al. (2019). In that study, a gradient transport model (GTM) was employed rather than DALES, but it used similar physical parameters for the landscape and the overlying atmosphere. For comparison between the studies, the same zones of influence as used in Batista et al. (2019) are examined herein, specifically 0%–25%, 0%–50%, and 0%–75%. Table 3 lists comparative results. To first order, the zones of influence between the DALES and GTM are simulated as having values of the same order of magnitude (rows 1 and 2). In more detail, the

![Figure 6](image)

**Figure 6.** Influence length $\lambda$ and horizontal shift $\delta$ for a zone of influence of 0%–63%. Results are plotted as a function of (a) sampling height, (b) wind speed, and (c) chemical lifetime. In panels (a–c), the lines are empirical fits to guide the eye.

| Model                                      | Physical and chemical processes                      | Zones of influence (m) |
|---------------------------------------------|------------------------------------------------------|------------------------|
|---------------------------------------------|------------------------------------------------------|------------------------|
| Large-eddy simulation (this study)          | –                                                    | 190  340  650         |
| Gradient transport model (Batista et al., 2019) | Reference case$^a$                                   | 150  700  2,350       |
| Pollution + sweep-ejection (20% dilution)   | Reference case$^a$                                   | 100  450  1,550       |

**Notes.** A species lifetime of 1630 s, representing isoprene, is used for all cases. The wind speed is fixed at 2 m s$^{-1}$. The sampling point is 20 m above the canopy. For comparison, a zone of influence of 63% in the terminology of Batista et al. (2019) is identical to the definition of influence length used herein (e.g., Table 2 and elsewhere).

$^a$The reference case corresponds to the parameters listed in Table S5 of Batista et al. (2019).
zones of influences for DALES compared to GTM are wider by a factor of 2 for 0%–25% yet more compact by a factor of 2–3 for 0%–50% and 0%–75%. Two interacting factors contribute to the differences. In the near field, horizontal advection plays a greater role in DALES than in GTM, leading to a wider zone of influence for 0%–25%. In the far field, the explicit treatment in DALES results in greater turbulent transport than is implicit in GTM, thus leading to a more compact zone of influence for 0%–50% and 0%–75% for DALES compared to GTM. The underprediction of turbulence by the GTM can be corrected to first order by including sweep injection (Batista et al., 2019). After this update, the results for GTM are closer to those of the DALES (Table 3, final row).

Once a value of $\lambda$ is obtained based on DALES for 0%–63% at a specific altitude, the following equation approximately predicts the value of $\lambda$ for other zones of $x%$:

$$L = -\lambda \ln[1 - x]$$

in which $x$ expressed as a fraction specifies the zone (e.g., 0.25, 0.50, or 0.75) and $L$ is the corresponding horizontal distance. The derivation of Equation 3 is presented in Section S5 of the Supplementary Information. Deviations of estimates by Equation 3 from the more detailed DALES results are presented in Table S3. The deviations are <40%, <15%, and <10% for zones of influence of 0%–25%, 0%–50%, and 0%–75%, respectively. Part of the deviation arises because Equation 3 omits the horizontal shift $\delta$.

4. Conclusions and Recommendations

The findings of this study lead to several conclusions and recommendations concerning sampling strategies by hovering UAVs of atmospheric species of different chemical lifetimes.

4.1. Recommendations for Sampling Height

Concentrations drop significantly with altitude as a result of chemical reactions and dispersion. For high- and intermediate-reactivity species, sampling near the surface is, therefore, recommended. This recommendation is germane to species for which dry deposition is unimportant. For species for which dry deposition is important, many complications are possible depending on the local heterogeneity of emission rates, wind speed, and upwind emissions. Future dedicated studies are needed to explore cases relevant to UAV sampling of species that undergo significant dry deposition.

For sampling over a landscape of heterogeneous emissions, the blending height increases with the length scale of heterogeneity. This relationship thus directly influences the highest suggested sampling height. The limit of this effect is the height of the planetary boundary layer. A typical forest has a heterogeneity scale of 200 m in the central Amazon, which has a simulated blending height of 210 m. As a point of comparison, the blending height increases to 700 m for a doubling in the heterogeneity scale to 400 m. The blending height also depends on the surface heat flux (i.e., induced atmospheric turbulence), and thus it can vary across the day and over different seasons. Below the blending height, the influence length and the horizontal shift of emissions from upwind forests increase for higher UAV sampling heights, faster horizontal wind speeds, and longer species chemical lifetimes.

For low-reactivity species that have emission rates that are sufficiently high to perturb near-surface concentrations, similar sampling strategies are suggested as those of high- and intermediate-reactivity species. For low-reactivity species of lower emission rates, near-surface sampling at a fixed location (e.g., as from a tower platform) can be representative of local to regional concentrations. When this scenario holds, the additional efforts required to make measurements by hovering UAVs are not expected to be well motivated, and tower measurements are recommended.

4.2. Recommendations for Sampling Duration

The turbulence analysis presented herein shows the importance of sufficient sampling duration, especially for high- and intermediate-reactivity species. A longer sampling duration reduces the inherent variability
caused by atmospheric turbulence at the spatiotemporal point of UAV sampling. Sampling durations of at least 10 min (high-reactivity species) and 5 min (intermediate-reactivity species) are adequate for averaging out the effects of atmospheric turbulence. This recommendation is, however, subject to other possible considerations related to species concentrations and analytical sensitivity of instrumentation. For example, a high-reactivity species might have a low atmospheric concentration, so a longer sampling duration might be necessary for detection. An alternative in this circumstance in some cases could be to focus on the product species rather than the parent species. Over the course of a day or between seasons, the sampling duration should also be adjusted in response to the strength of prevailing atmospheric turbulence.

Another consideration in real-world practice is that the sampling duration has an upper limit based on the battery capacity of the UAV (Stewart & Martin, 2020a). As an example, the maximum flight time is 30 min without payload and 17 min with a maximum payload of 5 kg for the medium-sized hovering UAV used in Batista et al. (2019). For comparison to these maximum flight times, the recommendation above varied from 5 to 10 min to average out the effects of atmospheric turbulence. A practical implication of these results, for example, is that the UAV used in Batista et al. (2019), which was equipped with a 2-kg VOC sampler for a flight duration of 25 min, could collect four samples during one flight when targeting a species of intermediate reactivity and two samples when targeting a species of high reactivity. Multiple sets of batteries can be used, and in this scheme the UAV can be relaunched, effectively achieving 50 min of flight time during each hour for as many hours as fresh batteries are available (Batista et al., 2019; Guimarães et al., 2019, 2020).

4.3. Recommendations Related to UAV-Induced Disturbance of Concentration Field

The perturbation in the atmosphere of the concentration distribution of a species because of UAV-induced turbulence and downdraft should be considered in the sampling strategy. These effects can downgrade the spatial resolution of a chemical species that can be resolved by a hovering UAV. Computation and smoke tests suggest that hovering UAVs can disturb the local atmosphere on order of 1 m around a small-sized UAV (i.e., <5 kg) (Alvarado et al., 2017; Prudden et al., 2016; Ventura Diaz & Yoon, 2018; Wolf et al., 2017) and <10 m for a medium-sized UAV (i.e., <25 kg) (Crazzolara et al., 2019; Hass et al., 2014; Lampert et al., 2020). Sampling over a forest canopy should be at least one disturbance length higher than the canopy (i.e., <10 m for a medium-sized UAV) to avoid copter-wake that might increase or decrease forest emissions. When near-field sampling is desired for scientific reasons, one possible approach is a downward extension of the sampling inlet by one disturbance length or longer (Shah et al., 2019). The present study, however, does not treat these near-field effects because the DALES treatment has a comparatively coarse resolution (i.e., 20 m). The implication is that the averaging kernel in the DALES analysis of a cube of 20 m is significantly larger than the disturbance field for the types of UAVs considered (i.e., take-off mass <25 kg). The UAV disturbance field, therefore, does not affect the results of the present study and simulation. Even so, for different atmospheric applications that seek better spatial resolution than 10 m, care must be taken in the sampling strategy to consider local disturbances caused by the hovering UAV.

4.4. Recommendations for Selection of UAV System

Selection of a specific hovering UAV for atmospheric chemical sampling can depend on the purpose. For sampling at high spatial resolutions, small UAVs are preferred because the UAV-induced disturbance increases with UAV size. For sampling of chemical species of low atmospheric concentrations, UAVs that have long flight endurance that permit longer sampling durations are preferred. Selection should also take into consideration the payload mass and size limits, the maximum flight altitude, and local civil aviation regulations.

Sampling strategies and recommendations by fixed-wing UAVs are a complementary topic that is recommended for future study. Fixed-wing and hovering UAVs can each be important for different applications and at times provide important complementary overlap (Table 1). A hovering configuration is preferred when the instrumentation or sampling require longer integration kernels for sufficient sensitivity or, if sensitivity is sufficient, when a time series of concentrations at single atmospheric position is desired. One governing guideline between a hovering UAV and a fixed-wing UAV is the following inequality: for a desired spatial resolution \(d\) and a required sampling or measurement time \(\tau\) (i.e., for instrumentation sensitivity),
then the UAV must have a horizontal speed of less than $d/r$. As one example, for a measurement that requires a sampling duration of 5 min and a spatial resolution of 10 m, the horizontal speed of the UAV must be less than 0.03 m s$^{-1}$. For comparison, typical fixed-wing UAVs have a minimum velocity of approximately 10 m s$^{-1}$ to avoid stall. For this kind of scenario (i.e., 0.03 < 10), a hovering UAV is therefore preferred. Many contrasting scenarios that recommend the use of fixed-wing UAVs are also easily formulated. The use of both types of UAVs in a combined strategy is a synergistic possibility that is important for future study and in some cases could achieve unique insights.

In summary, the results presented herein provide important recommendations for controlled and accurate UAV sampling of species concentration and transport in the atmospheric boundary layer under fair-weather conditions over tropical forests. A caution is that an extension of the quantitative results of the current simulation setup to other biomes such as boreal and temperate forests may not be directly applicable because of markedly different input parameters for those biomes (e.g., wind speed, surface heat flux, and species lifetimes). Even so, many of the qualitative findings of this study should still be recognizable for other biome types. Considerations of the relationship between atmospheric species concentrations sampled by a hovering UAV and the possible underlying landscape emissions of that species, especially in the case of spatial heterogeneity of the emission rates, should be combined with the variables discussed herein in order to optimize flight and sampling strategies over different types of landscapes and in response to daily microscale meteorology.

**Data Availability Statement**

The numerical experiments were performed using the Dutch Atmospheric Large Eddy Simulation, version 4.1 (Heus et al., 2010). It can be downloaded from https://doi.org/10.7910/DVN/VXCM5R. The DALES code, the numerical settings, benchmarks, and study results are available: https://doi.org/10.7910/DVN/VXCM5R.

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