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Modelling the effect of the 2018 summer heatwave and drought on isoprene emissions in a UK woodland

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Abstract
Projected future climatic extremes such as heatwaves and droughts are expected to have major impacts on emissions and concentrations of biogenic volatile organic compounds (bVOCs) with potential implications for air quality, climate and human health. While the effects of changing temperature and photosynthetically active radiation (PAR) on the synthesis and emission of isoprene, the most abundant of these bVOCs, are well known, the role of other environmental factors such as soil moisture stress are not fully understood and are therefore poorly represented in land surface models. As part of the Wytham Isoprene iDirac Oak Tree Measurements campaign, continuous measurements of isoprene mixing ratio were made throughout the summer of 2018 in Wytham Woods, a mixed deciduous woodland in southern England. During this time, the United Kingdom experienced a prolonged heatwave and drought, and isoprene mixing ratios were observed to increase by more than 400% at Wytham Woods under these conditions. We applied the state-of-the-art FORest Canopy-Atmosphere Transfer canopy exchange model to investigate the processes leading to these elevated concentrations. We found that although current isoprene emissions algorithms reproduced observed mixing ratios in the canopy before and after the heatwave, the model underestimated observations by ~40% during the heatwave–drought period implying that models may substantially underestimate the release of isoprene to the atmosphere in future cases of mild or moderate drought. Stress-induced emissions of isoprene based on leaf temperature and soil water content (SWC) were incorporated into current emissions algorithms leading to significant improvements in model output. A combination of SWC, leaf temperature and rewetting emission bursts provided the best model-measurement fit with a 50% improvement compared to the baseline model. Our results highlight the need for more long-term ecosystem-scale observations to enable improved model representation of atmosphere–biosphere interactions in a changing global climate.

KEYWORDS
canopy exchange modelling, climate change, heatwave–drought, isoprene emissions, isoprene mixing ratios, rewetting, soil water content

1 | INTRODUCTION

The biogenic volatile organic compound (bVOC), isoprene (C_5H_8), has important impacts on atmospheric composition and chemistry due to its relative abundance and high reactivity (e.g. Fuentes et al., 2000; Laothawornkitkul, Taylor, Paul, & Hewitt, 2009). Chemical reactions involving isoprene lead to the production of secondary pollutants, for example, ozone (O_3) and secondary organic aerosol (SOA), which are also short-lived climate forcers. Isoprene also indirectly affects climate by reducing the oxidative capacity of the atmosphere, hence enhancing the atmospheric lifetime of climate active gases such as methane (CH_4; see e.g. Pike & Young, 2009). Increased isoprene emissions could potentially lead to up to a 50% change in surface ozone concentrations (Pike & Young, 2009) but the sign of change depends on geographical location and atmospheric composition, in particular on the concentrations of the oxides of nitrogen ($NO_x = NO + NO_2$). The large quantities of isoprene emitted into the atmosphere make it a major source of SOA, although aerosol yield from isoprene depends on a number of factors including levels of organic aerosol loading and NO_x concentrations (Carlton, Wiedinmyer, & Kroll, 2009). SOA has an indirect impact on climate through changing cloud optical properties (Carslaw et al., 2010; Unger, 2014). Isoprene and other bVOCs have been estimated to have a net negative radiative forcing which offsets the positive radiative forcing of anthropogenic volatile organic compounds (Unger, 2014). Isoprene could therefore play an important role in future climates through its regulation of atmospheric chemistry and formation of secondary pollutants, although its overall climate impact is minor compared to greenhouse gases such as CO_2, and remains uncertain (Arneth et al., 2010).

More than 90% of global isoprene is emitted by terrestrial vegetation (Guenther et al., 2006) at a rate primarily dependent on vegetation type (with forests contributing ~80% of global annual emissions) but also on environmental conditions such as temperature, solar radiation, atmospheric CO_2 concentration and soil moisture (Guenther et al., 2006 and references therein; Laothawornkitkul et al., 2009). Several hypotheses have been proposed to explain why some plants synthesize and emit isoprene, the best supported being that it prevents cellular damage caused by heat and oxidative stress (e.g. Sharkey, 2000; Vickers, Gershenzon, Lerdau, & Loreto, 2009). Hence, emissions increase under high temperature and insolation.

During periods of water stress, however, physiological processes such as stomatal conductance, photosynthesis rate and respiration are reduced, resulting in a decrease in plant productivity (Keenan, Sabate, & Gracia, 2010). Isoprene emissions are closely coupled with photosynthesis and so reductions in plant photosynthetic capacity as a result of water stress would be expected to lead to a decrease in isoprene emissions by reducing the supply of carbon available for its synthesis. Indeed, studies have observed decreases in isoprene emission rates of between 40% and 60% under severe drought conditions (e.g. Brilli et al., 2007; Brüggemann & Schnitzler, 2002; Lerdau & Keller, 1997; Pegoraro et al., 2004).

However, an increase in emissions under drought has also been reported (Brilli et al., 2007; Loreto & Schnitzler, 2010; Rennenberg et al., 2006; Sharkey & Loreto, 1993) suggesting that water stress can decouple isoprene emission from photosynthesis, possibly because isoprene emissions are unaffected by decreasing stomatal conductance (Centritto, Brilli, Fodale, & Loreto, 2011; Pegoraro et al., 2004; Tingey, Evans, & Gumpertz, 1981). Experiments using ^{13}C labelling have shown that isoprene can be produced from older pools of stored carbon when photosynthetic gas exchange is reduced by drought (e.g. Brilli et al., 2007).

The net impact of soil water stress on isoprene emissions remains uncertain due to these competing effects. It is likely that the apparently contradictory responses observed in laboratory experiments are due to differences in the severity of the applied drought and the tolerance of different plant species to water stress, with severe drought, in which the soil water content (SWC) falls below the permanent wilting point, leading to a decline in isoprene emissions and mild-to-moderate drought having either no impact or leading to an increase. Niinemets (2010) developed a conceptual model in which the initial increase in leaf temperature that occurs as stomata close in response to a decline in soil moisture stimulates isoprene synthesis and emissions, leading to the observed decoupling of emissions from gas exchange rates. Evidence for this model was later provided by Potosnak et al. (2014) who observed this behaviour at the onset of a prolonged drought in the Ozarks, an oak-dominated mid-latitude forest.

An additional complexity is the response of isoprene emission rates to rewetting. Sharkey and Loreto (1993) and Penuelas Filella Seco and Llusia (2009) observed a substantial increase in isoprene emissions from seedlings after rewetting but this effect has not been observed in all experiments. Pegoraro et al. (2004) reported a lag of about a week between declining soil moisture and changes in isoprene emission rates most likely the result of plants having to adjust to the restoration of the photosynthetic carbon source for isoprene synthesis and emission.

The effect of temperature and solar radiation on isoprene emissions are relatively well understood and emissions estimates from land surface models have been shown to capture observed diurnal variations in fluxes and concentrations reasonably effectively across a range of ecosystems (e.g. Guenther et al., 2012; Zimmer et al., 2000). Unlike temperature and solar radiation, there is no direct impact of soil water deficit and soil rewetting on isoprene emissions and these are therefore not well represented in coupled land surface-atmosphere models although numerous studies have shown their importance to emission rates and atmospheric composition (e.g. Emmerson, Palmer, Thatcher, Haverd, & Guenther, 2019; Guenther et al., 2006; Jiang et al., 2018; Sindelarova et al., 2014).

Rising levels of CO_2 and future changes in climate, such as increasing temperature and altered patterns of precipitation, can thus be expected to change isoprene emissions from the current estimated 450–600 Tg C/year (Arneth, Monson, Schurgers, Niinemets, & Palmer, 2008; Guenther et al., 2006, 2012). Heald et al. (2009) projected increases of as much as ~190 Tg C/year in global isoprene emissions due to a temperature increase of 2.3°C by 2100 but also showed that a decrease in isoprene emissions due to increasing CO_2 concentrations could off-set this temperature effect almost entirely.

Most studies to understand the effect of combined heatwaves and drought on isoprene emissions have been laboratory-based experiments which permit close control of environmental factors such as temperature, photosynthetically active radiation (PAR) and soil moisture but make use of saplings (e.g. Brilli et al., 2007), seedlings or young plants (e.g. Pegoraro et al., 2005) and are thus not representative of real-world forest environments. There are limited observations of isoprene emissions during drought in natural ecosystems (e.g. Emmerson et al., 2019; Potosnak et al., 2014; Seco et al., 2015) which are necessary to enable the development of robust parameterizations in emission models.

In the summer of 2018, the United Kingdom (UK), in common with most of northern and central Europe, experienced a prolonged drought and heatwave event. The UK Met Office officially declared heatwave conditions starting on June 22 which persisted to August 8 in southern England. Records from the UK Met Office show that the 2018 summer mean temperature over the UK as a whole was ~2.0°C above the 1961–1990 average, making the summer of 2018 the joint warmest on record (Regional Values, 2019). The mean temperature over southern England was 17.7°C, ~2.4°C warmer than the 1961–1990 average.

Under future climate scenarios, droughts and heatwaves that are currently thought of as anomalous (such as the one that occurred in 2018) are expected to increase in frequency (IPCC, 2013; Thornton, Ericksen, Herrero, & Challinor, 2014) with the UK Met Office predicting that the UK may experience such conditions every other year by 2050 (e.g. UK Extreme Events—Heatwaves, 2019). Given the role of isoprene and other BVOCs in the formation of short-lived climate forcers and SOAs, the potential impacts of these changes in climate on isoprene emission rates and therefore on atmospheric composition, air quality and climate (Pacifico, Harrison, Jones, & Sitch, 2009; Sanderson, Jones, Collins, Johnson, & Derwent, 2003) must be better understood.

The combined heatwave and drought (heatwave–drought) and rewetting episodes, which occurred during the Wytham Isoprene iDirac Oak Tree Measurements (WIsDOM) campaign in Wytham Woods in 2018, offered a unique opportunity to quantify the potential effect of future climate change on isoprene emissions in a natural environment. This study uses a state-of-the-art canopy model to explore the observed effects of heat and drought stress, and soil rewetting on isoprene emissions and mixing ratios in a temperate mixed deciduous woodland.

2 | MATERIALS AND METHODS

2.1 | Site description

The WIsDOM campaign took place at Wytham Woods (51°46′23.3″N 1°20′19.0″W, 160 m a.s.l.), located ~5 km NW of the centre of Oxford in SW England, between May and October 2018. The forest has been owned and maintained by the University of Oxford as a site of special scientific interest since 1942 and has been part of the UK Environmental Change Network (ECN) since 1992. The forested area is made up of patches of ancient semi-natural woodland, secondary woodland, and modern plantations and is dominated by European Ash (*Fraxinus excelsior*—26%), Sycamore (*Acer pseudoplatanus*—18%), European Beech (*Fagus sylvatica*—11%) and English Oak (*Quercus robur*—7%; Kirby et al., 2014). The remainder of the forest comprises other broadleaf trees and shrubs. *Q. robur* (~95%) and *A. pseudoplatanus* (~5%) are the main contributors to the isoprene budget at Wytham Woods (Bolas, 2020). The forest has largely been undisturbed over the last 40–100 years (Morecroft, Stokes, Taylor, & Morison, 2008; Thomas et al., 2011) and as a consequence the age range of mature trees in Wytham Woods is large—from 40 to >150 years. The climate in Oxfordshire can be classified as warm temperate with rainfall occurring all year round. The 1981–2010 average summer temperature ranges between 18 and 20°C and average rainfall is ~600–700 mm/year.

2.2 | Measurement campaign

Continuous measurements of isoprene mixing ratios were made approximately every 20 min at four heights in the forest canopy between June and October 2018 during the WIsDOM campaign. Inlets to two dual-channel iDiracs (see Bolas et al., 2019 for a full description of the instrument design and deployment) were located at 15.55m (top of canopy), 13.17 m (mid-canopy), 7.26 m (trunk height) and 0.53 m (near surface) alongside a mature *Q. robur* of ~16 m height. Measurements at the trunk and near-surface levels did not start until July. The iDirac has a detection limit of ~38 ppt with an instrument precision of ±11% (Bolas et al., 2019).

Hourly measurements of temperature, PAR, relative humidity, soil moisture at a depth of 20 cm, wind speed and direction, and atmospheric pressure were obtained from the Upper Seeds automatic weather station located in a small clearing ~480 m from the site of the isoprene observations. We used 30 min averages of the measurements made between 1 June and 30 September in our model analysis. This covers the full extent of peak growth with roughly equal periods before, during and after the heatwave–drought. For full details of the WIsDOM campaign, readers are referred to Ferraci, Bolas, and Harris (2020).

2.3 | Model description

We applied the FORest Canopy-Atmosphere Transfer (FORCAsT) 1D model of biosphere–atmosphere exchange to simulate the processes of biogenic emissions, chemical production and loss, vertical mixing, advection and deposition within and above the canopy at Wytham Woods. A detailed description of the FORCAsT model can be found in Ashworth et al. (2015), so here we focus only on those elements of the model configuration relevant to this study. We subdivided the 40 model levels into 10 between the ground surface and trunk height, and a further 10 within the crown space to ensure that observation heights aligned as closely as possible with the mid-point of a model level.

Vertical transport in FORCAsT is based on a modified k-theory of vertical turbulent diffusion (Blackadar, 1979; Raupach, 1989). In-canopy and above canopy mixing are simulated following Baldocchi (1988) and Gao, Wesely, and Doskey (1993), respectively. The simulated exchange of heat and trace gases is further improved by constraining the friction velocity (u*) and the standard deviation of the vertical wind component (σ_w) following Bryan et al. (2012). As u* and σ_w were not measured at Wytham, we estimated each from the horizontal wind speed (u) following Makar et al. (2017), Equation (1), and Shuttleworth and Wallace (1985), Equation (2), respectively:

$$u* = \frac{u \times K}{\ln\left(\frac{h_c}{Z_o}\right)}, \tag{1}$$

$$\sigma_w\left(\frac{z}{h_c}\right) = \begin{cases} 1.25u* & \text{for } \frac{z}{h_c} > 1.0 \\ u*\left[0.75 + 0.5 \times \cos\left(\pi\left(1 - \frac{z}{h_c}\right)\right)\right] & \text{for } \frac{z}{h_c} < 1.0 \end{cases}, \tag{2}$$

where h_c is the height of top of canopy (18 m), Z_o is the roughness length (assumed 0.1*h_c), u is the mean horizontal wind speed at height z and K is von Karman's constant (0.4).

In FORCAsT, isoprene is produced through emissions from foliage in the crown space and lost through oxidation reactions initiated by the OH and NO_3 radicals and O_3, and through deposition to the soil (following Stroud et al., 2005). The concentration of isoprene at each level in the canopy depends on these production and loss processes as well as fluxes into and out of that layer. Previous studies (e.g. Bryan et al., 2012; Guenther et al., 2006 and references therein) have shown that for moderate height canopies such as that at Wytham Woods, canopy residence times are sufficiently short that little isoprene is lost through oxidation within the canopy. Hence, concentrations are primarily dependent on emission rates when considered over periods greater than turbulent timescales (≤1 s to min). FORCAsT employs a half-hourly timestep. Our simulations therefore focused on the emissions of isoprene, which are calculated in FORCAsT by summing the contributions from 10 leaf angle classes in each crown-space model level, following the algorithms of Guenther et al. (1995):

$$\mathrm{ER} = \mathrm{LAI} \cdot \varepsilon \cdot \gamma_{iso}, \tag{3}$$

where ER is the total emission rate (mg m^{-2} hr^{-1}), LAI (m^2/m^2) is the leaf area index and ε is a site- and species-specific emission factor (1.20 mg m^{-2} hr^{-1} for *Q. robur*; Visakorpi et al., 2018) which represents the emission rate of isoprene into the canopy at standard conditions of 30°C and 1,000 µmol m^{-2} s^{-1}. LAI was taken as the maximum reported for the site (3.6 m^2/m^2; Herbst, Rosier, Morecroft, & Gowing, 2008) throughout this study which coincides with the period of peak growth. γ_{iso} is a dimensionless emission activity factor that accounts for changes in emission rates due to deviations from these standard conditions, with:

$$\gamma_{iso} = C_L C_T, \tag{4}$$

where C_L and C_T are the light and temperature dependence of isoprene emission rates, respectively, and are given by:

$$C_L = \frac{\alpha C_{L1} \mathrm{PAR}}{\sqrt{1 + \alpha^2 \mathrm{PAR}^2}}, \tag{5}$$

where α (=0.0027) and C_{L1} (=1.066) are empirical coefficients from Guenther et al. (1995).

$$C_T = \frac{\exp \frac{C_{T1(T-T_s)}}{RT_s T}}{1 + \exp \frac{C_{T2(T-T_m)}}{RT_s T}}, \tag{6}$$

where T is the leaf temperature (K), T_s is the temperature at standard conditions (i.e. 303 K), R is the ideal gas constant (=8.314 J K^{-1} mol^{-1}), C_{T1} (=95,000 J/mol), C_{T2} (=230,000 J/mol) and T_M (=314 K) are empirical coefficients determined by Guenther et al. (1995). Leaf temperature is calculated from measured air temperature in FORCAsT using a canopy energy balance.

Equations (3)–(6) describe the default model set-up (hereafter referred to as BASE). We conducted a series of experiments introducing stress-induced emissions, achieved by further modifying the activity factor to account for extreme temperature and drought conditions. In these experiments, described below, γ_{iso} was calculated as follows:

$$\gamma_{iso} = C_L C_T \gamma_X, \tag{7}$$

where γ_X is an additional environmental activity factor and X denotes the environmental condition affecting isoprene emission rates in each experiment explained in detail below.

2.4 | Model experiments

2.4.1 | BASE

FORest Canopy-Atmosphere Transfer was configured using site-specific canopy parameters and isoprene emission factors and driven with meteorology measured at Wytham Woods during the WIsDOM campaign. Isoprene emission rates for each model level were calculated within the model using Equations (3)–(6). Comparison of modelled isoprene mixing ratios against observations from the iDirac instruments at four heights within the canopy showed good agreement in both diurnal profile and magnitude before and after the heatwave–drought. However, during the heatwave–drought period, the model substantially underestimated isoprene mixing ratios. The results from this simulation are described in more detail later.

We therefore performed three subsequent experiments, introducing $\gamma_{X,}$ to explore the possible environmental factors driving the sharp increase in observed isoprene concentrations that the model was unable to account for using the standard emissions algorithms. In all three experiments, model configuration and driving meteorology remained unchanged from BASE; the only difference was the change to the isoprene activity factor described below.

2.4.2 | BASE+LFT

During periods of drought stress, there is an increase in leaf temperature due to a reduction in transpiration rate as the plants attempt to conserve water (Zandalinas, Mittler, Balfagón, Arbona, & Gómez-Cadenas, 2018). Niinemets (2010) and Potosnak et al. (2014) hypothesized that this increase in leaf temperature is the cause of observed increases in isoprene emissions during mild-to-moderate drought stress. Here we test whether increases in leaf temperature explain the observed changes in isoprene mixing ratios observed during WisDOM by modifying γ_X against leaf temperature (hereafter referred to as LFT) with γ_{LFT} defined as follows:

$$\gamma_{LFT} = \begin{cases} 1 & T < T_{95} \\ \frac{T - T_s}{T_{95} - T_s} & T \geq T_{95} \end{cases}, \tag{8}$$

where T (K) is the leaf temperature, T_s (297 K) represents the standard conditions for leaf temperature (Guenther et al., 2006) and T_{95} is the 95th percentile of the seasonal leaf temperature which represents the threshold temperature above which we assume heat-induced emissions occur.

2.4.3 | BASE+SWT

Under heatwave–drought conditions, it would be expected that reduced SWC and unusually high temperatures affect emissions rates simultaneously. This experiment therefore combines the effect of soil water deficit and leaf temperature on isoprene emissions into a single environmental activity factor, γ_{SWT} calculated as follows:

$$\gamma_{SWT} = \begin{cases} 1 & \text{for } \theta > \theta_c \\ \left[\frac{(\theta - \theta_w)}{\theta_c - \theta_w}\right]^q \times [\gamma_{LFT}] & \text{for } \theta_w < \theta \leq \theta_c \end{cases}, \tag{9}$$

where θ (m^3/m^3) is the volumetric soil moisture, θ_w is the wilting point (0.15 m^3/m^3 following Jiang et al., 2018), θ_c (0.22 m^3/m^3) is a critical soil moisture content above which we observe no effect of water stress on isoprene emissions and q is a site-specific empirical factor describing the non-linearity of the effects of soil water stress on tree physiological processes. A range of q values have been tested for different plant functional types (e.g. see Egea, Verhoef, & Vidale, 2011). Here a value of 0.40 provided the best fit to observations. γ_{LFT} is defined in Equation (8).

2.4.4 | BASE+RWT

This experiment investigates whether the burst of isoprene emissions observed following rewetting after drought in laboratory studies is seen at the ecosystem scale. The environmental activity factor, γ_{RWT}, is a modification of Equation (9) such that during periods defined as rewetting (days within the heatwave–drought period for which SWC exceeds that of the previous 10 days), γ_{RWT} is given by:

$$\gamma_{RWT} = \gamma_{SWT} \times 1.30, \tag{10}$$

that is, a 30% increase in isoprene emissions following soil rewetting.

3 | RESULTS

Here we present a comparison of continuous measurements of isoprene mixing ratios at all four iDirac inlet levels against the output from the nearest model level. For the top and middle of the canopy, we use half-hourly averages of both modelled and observed data covering the period June 1 to September 30 for this comparison; measurements are only available for the trunk and near-surface levels between July 6 and September 30. Statistical values reported in this section were restricted to isoprene mixing ratios between 0600 LT and 1900 LT coinciding with daylight hours when isoprene emissions occur, in keeping with previous studies (e.g. Potosnak et al., 2014; Seco et al., 2015). The data are presented in full as time series, and then summarized to show goodness of fit using scatter plots and a Taylor diagram (Taylor, 2001). The Taylor diagram provides a way to demonstrate the simultaneous variation of three model performance statistics: correlation coefficient (r^2), normalized standard deviation (*SD*) and centred root-mean-square error (RMSE). Output from an ideal model would show the same r^2, *SD* and RMSE as the observations. Therefore, the closer a model's summary statistics are to that of the observations on the Taylor diagram, the better its performance. Results are first presented for the BASE simulation (i.e. the default model set-up) and then for each experiment. Model performance statistics for the top of the canopy is presented here while those for the other levels can be found in the Supplementary Information. The grey shaded region on all figures indicates the heatwave–drought period as defined by the UK Met Office for southern England and the dashed white line the start of rewetting.

3.1 | Meteorological conditions

Figure 1a–c shows PAR, temperature, volumetric SWC and precipitation measured at the ECN station in Wytham Woods for the study period. Following a wet April in which rainfall was ~120% of the 1981–2010 mean (Monthly, seasonal and annual summaries 2018, 2019), SWC declined steadily from near field capacity (at 0.46 m^3/m^3)

at the start of June to 0.16 m^3/m^3 (just above the wilting point of 0.15 m^3/m^3 for this site) at the peak of the heatwave–drought in July. A few low-intensity rainfall events (total precipitation <0.2 mm) with negligible effect on SWC were recorded prior to the heatwave–drought. Rainfall during the heatwave–drought, on July 20 (3 mm) and July 27 (11.1 mm), led to increases in soil moisture and the 're-wetting period' extended from 20 July to 8 August as a result. The Standardized Precipitation Index (McKee, Doesken, & Kleist, 1993), used to characterize the severity of meteorological droughts, indicates Wytham Woods experienced a moderate drought in July (https://eip.ceh.ac.uk/apps/droughts/), consistent with in-situ SWC measurements. After 8 August (the official end of the heatwave period), rainfall frequency and intensity increased with a corresponding increase in soil moisture.

The average temperature recorded at Wytham Woods was 17.5°C for the entire measurement period (1 June–30 September), but 19.6°C during the heatwave (22 June–8 August). The diurnal temperature ranged from an average of 11.8°C at night to 21.3°C during the day for the whole season but increased sharply during the heatwave, with mean night-time and daytime temperatures of 13.5 and 25.2°C, respectively. For the same June to September period, climatological (1993–2015) temperature averaged 15.8°C with a diurnal range of 10.2–18.9°C. Compared to the long-term average, the 2018 summer at Wytham Woods was 1.7°C warmer mainly due to a 3.0°C increase in temperature during the heatwave–drought. The maximum temperature recorded at Wytham Woods during the 2018 heatwave–drought (30.6°C) was, however, lower than the climatological maximum (32.2°C). Average PAR increased from 781 W/m^2 before the heatwave–drought to 1,277 W/m^2 during it, reflecting longer and more intense periods of sunshine associated with the underlying high pressure conditions of the heatwave period.

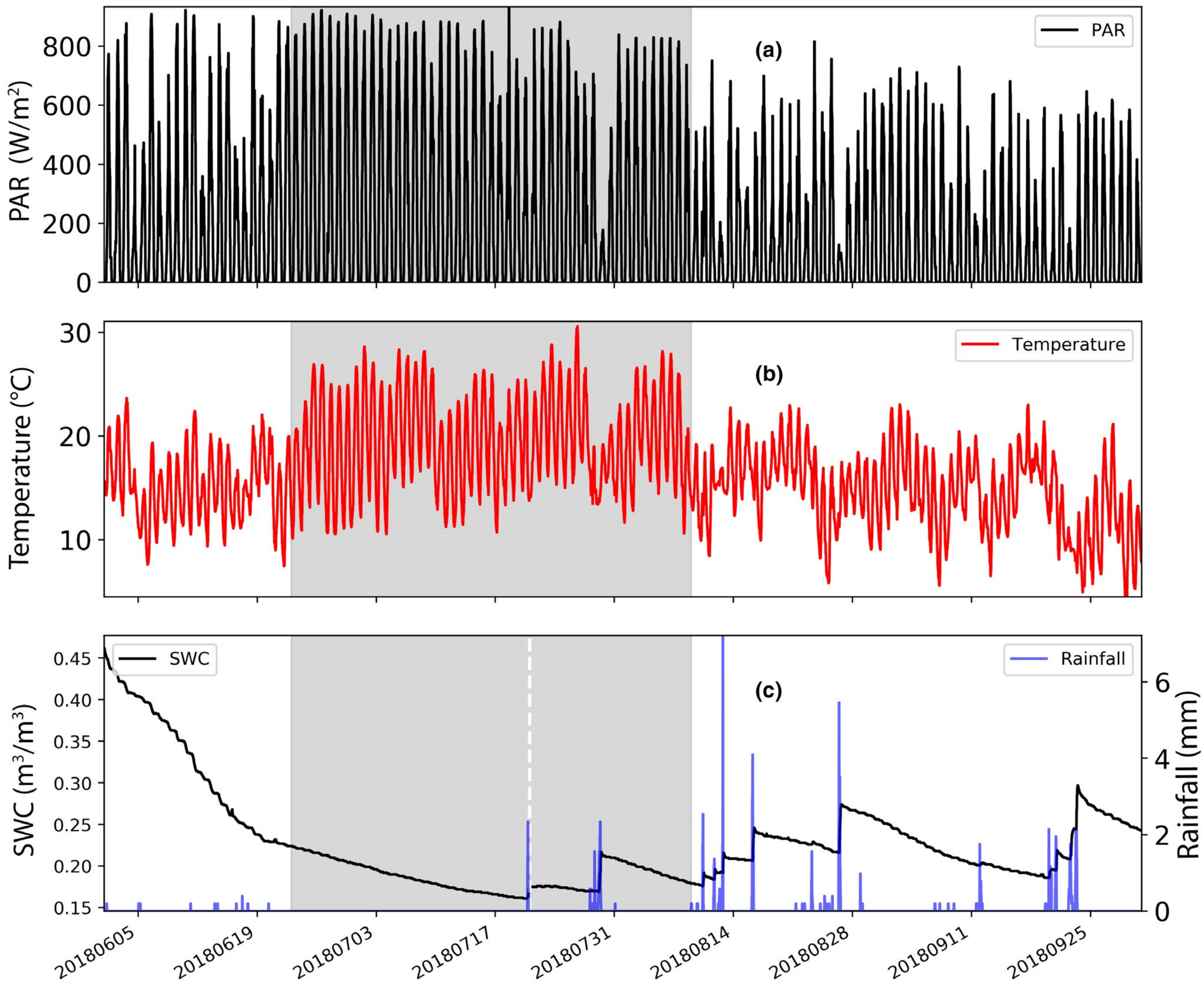

FIGURE 1 Meteorological data taken from the Wytham Woods Automatic Environmental Change Network station: (a) Photosynthetically active radiation (PAR), (b) 2 m air temperature, (c) soil water content (SWC; black) and total daily rainfall (blue). The grey shaded area indicates the start and end of the heatwave–drought while the white dashed line indicates the start of the rewetting period (20 July–8 August)

3.2 | Base model simulation

As isoprene emission rates are predominantly determined by light and temperature, BASE reliably reproduces the diurnal cycle of isoprene concentrations at each of the inlet levels (Figure 2a–d). Average modelled mixing ratios outside of the heatwave–drought are in good agreement with those observed (0.44 ppb vs. 0.37 ppb at the top of the canopy, 0.24 ppb vs. 0.18 ppb at mid-canopy level, 0.17 ppb vs. 0.15 ppb at trunk level and 0.09 ppb vs. 0.11 ppb near the surface), with no apparent systematic bias, suggesting that the emission factor, ε, is appropriate for the site. However, FORCAsT underestimates concentrations at all levels during the heatwave–drought by an average of 40% leading to a total underestimation of ~25% over the entire season. During the heatwave–drought, the average isoprene mixing ratio measured at the top of the canopy was 1.97 ppb (i.e. >4 times that outside the heatwave period) but only 1.12 ppb in BASE. Similar results were obtained at the other levels for model versus observations (1.01 ppb vs. 0.60 ppb at mid-canopy level, 0.84 ppb vs. 0.49 ppb at trunk level and 0.58 ppb vs. 0.15 ppb near the surface). Following the two rewetting episodes in July, average observed isoprene mixing ratios increased to 2.05 ppb, while modelled isoprene was nearly a factor of 2 lower at 1.12 ppb for that period. There was a 48%, 44% and 70% underestimation in the model at the mid-canopy, trunk and near-surface levels, respectively, following the rewetting events. These systematic discrepancies show that the emission burst observed following rewetting is unaccounted for in current emissions algorithms.

The time series of the difference between modelled and observed isoprene mixing ratios at the top of the canopy for BASE (Figure 3a) highlights the relatively poor skill of the standard emissions algorithms throughout the 7 week heatwave–drought

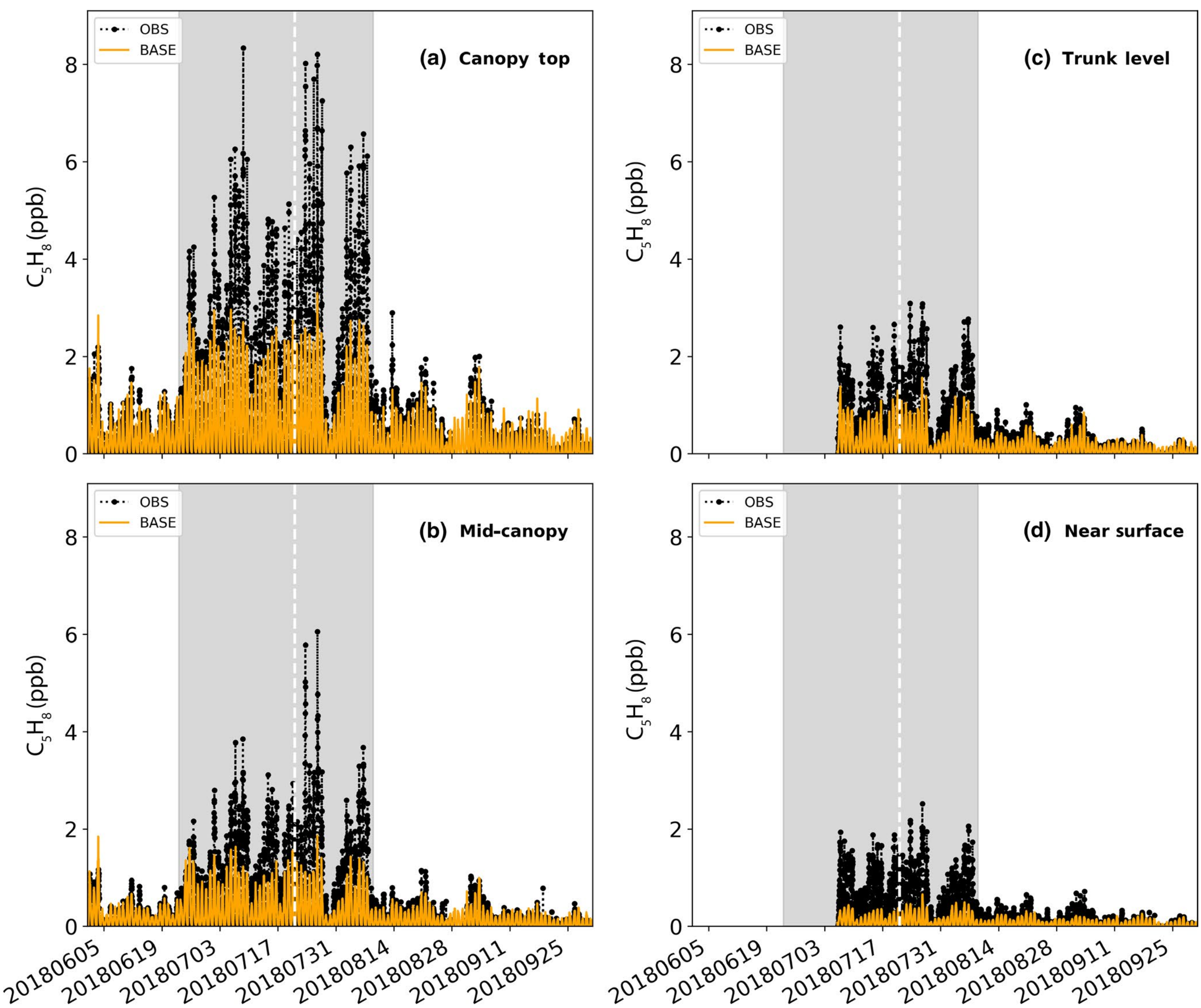

FIGURE 2 Observed (black) and modelled (BASE; orange) isoprene mixing ratios at the WIsDOM site at (a) the top of the canopy (~15.6 m), (b) mid canopy (~13.5 m), (c) trunk height (~7.1 m) and (d) near the surface (~0.8 m). Observations of isoprene mixing ratios at the trunk and near-surface levels started on 6 July

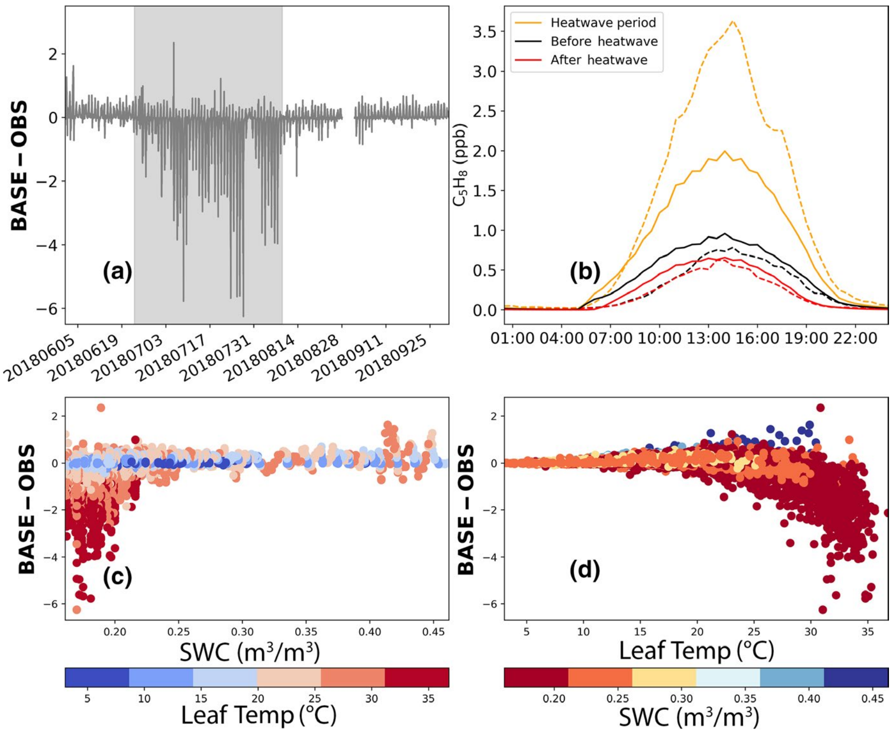

FIGURE 3 (a) Difference (in ppb) between model (BASE) and observed (OBS) isoprene mixing ratio at the top of the canopy for the BASE simulation for the entire season (1 June–30 September 2018). Note that negative values indicate periods when the model underestimates concentrations while positive values indicate an overestimation. (b) Diurnal profiles of isoprene mixing ratios at the top of the canopy before heatwave–drought (black), during the heatwave–drought (orange) and after the heatwave–drought (red). Model values are solid lines while observed values are dashed lines. Scatter plots of difference in mixing ratio versus (c) soil water content (SWC) coloured by temperature and (d) leaf temperature coloured by SWC

(shaded region). The average diurnal profiles of isoprene mixing ratios before, during and after the heatwave–drought presented in Figure 3b further confirm the good performance of BASE before and after the heatwave and the substantial underestimation during the heatwave. Figure 3c,d explores the relationship between these differences and the possible environmental drivers: SWC and temperature. Figure 3c points to a soil moisture threshold with isoprene mixing ratios (and therefore emissions) independent of SWC above ~0.22 m^3/m^3 but increasing rapidly as SWC drops further. This is in keeping with the concept of a critical SWC used in modelling both photosynthesis and isoprene emissions in previous work (e.g. Emmerson et al., 2019; Guenther et al., 2006; Keenan et al., 2010), although we see an increase rather than decrease as SWC declines below this threshold, similar to that reported under moderate drought stress by Potosnak et al. (2014). Figure 3d suggests a similar but less pronounced response to high temperatures (>20°C). We found no significant relationship between PAR and the difference between modelled and measured isoprene mixing ratios and conclude that high temperature and low SWC are the key drivers of the apparent stress-induced enhancement in isoprene emissions.

3.3 | Results of modelling experiments

Figures 2 and 3 show clearly that BASE underestimated isoprene concentrations during the heatwave–drought and at other times when isoprene levels in the canopy were high. In this section, we present the results of our model experiments exploring the addition of stress-induced emissions and compare them to the performance of BASE over the entire season. As for BASE, model performance statistics are similar for all levels for each experiment. We therefore present only statistics for top of the canopy here; statistics for the other levels are given in Table S1 in the Supporting Information.

3.3.1 | BASE+LFT

Modifying the isoprene activity factor when leaf temperature exceeds the 95th percentile (γ_{LFT}) reduces the net underestimation during the heatwave–drought but, as shown in Figure 4a,e, FORCAsT still substantially underestimates observed mixing ratios throughout this period. The average modelled isoprene mixing ratio is 1.26 ppb during the heatwave–drought (~35% lower than observed) and 0.76 ppb (25% too low) over the entire season. This tendency towards underestimation can be seen clearly in Figure 5b,f (most of the points lie below the 1:1 line) as can the improvement over the performance of BASE (shown in Figure 5a,e). Figure 6 further confirms that the use of a temperature-induced enhancement (γ_{LFT}) in isoprene emissions improves the overall fit to measurements. The RMSE of modelled mixing ratio is reduced (from 0.60 in BASE to 0.57 in BASE+LFT), reflecting a slightly improved accuracy during the heatwave–drought. The normalized standard deviation (0.61 in BASE vs. 0.66 in BASE+LFT) indicates that the model is also better able to reproduce the variability seen in the observed concentrations although still tending to underestimate. It should be noted that the correlation between modelled and observed isoprene is very good (>0.9) for all simulations as the strong dependency of isoprene emissions on temperature and PAR is well captured by the standard emissions algorithms (Equations 3–6) included in BASE. Figure 6 shows that although BASE+LFT improves model reproduction of isoprene mixing ratios, it is still unable to

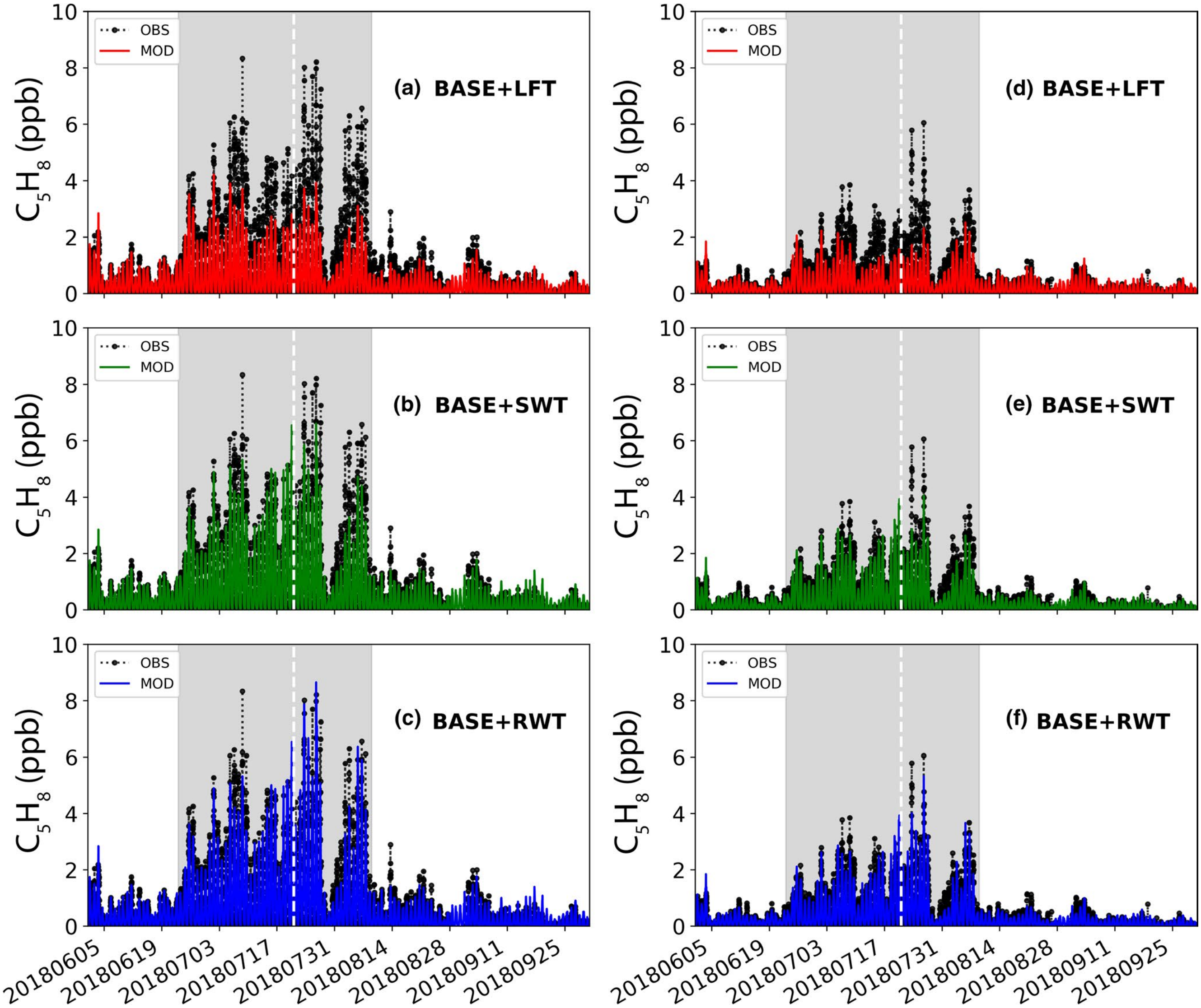

FIGURE 4 Observed (OBS) and modelled (MOD) isoprene mixing ratios at the top (15.6 m; a–c) and middle (13.5 m; d–f) of the canopy. Observations are shown in black and model results in red (BASE+LFT), green (BASE+SWT) and blue (BASE+RWT). Figure S2 in the Supporting Information shows similar results for the trunk and near-surface levels

account for the high concentrations during the heatwave–drought and suggests that other factors are responsible for the increase in isoprene concentration during this period.

3.3.2 | BASE+SWT

This experiment accounted for the simultaneous effect of heat and water stress. As shown in Figure 4b,e, there is a clear improvement in the model's estimation of isoprene mixing ratios during the heatwave–drought period compared to both BASE and BASE+LFT and this is further confirmed by Figure 5c,g, in which most points lie along or close to the 1:1 line. Figure 5c,g also shows that BASE+SWT consistently underestimates when observed mixing ratios are high (>5 and >3 ppb at the top and middle of the canopy, respectively). The mean modelled isoprene mixing ratio at the top of the canopy is 1.87 ppb, just ~5% lower than the observed value of 1.97 ppb. There are no periods of consistent model bias, rather FORCAsT underestimates isoprene concentrations periodically through the heatwave period, resulting in the standard deviation <1.0 in Figure 6. Referring to Figure 1b, it can be seen that these periods of underestimation correspond to rewetting periods following rainfall events. The average modelled mixing ratio during the rewetting period was 1.73 ppb compared to the observed value of 2.05 ppb. This constitutes ~15% underestimation compared to observed values but ~35% increase (improvement) over the 1.12 and 1.11 ppb estimated in BASE and BASE+LFT, respectively.

3.3.3 | BASE+RWT

The final experiment included an additional 30% enhancement of the environmental activity factor following soil rewetting (γ_{RWT}) and, as

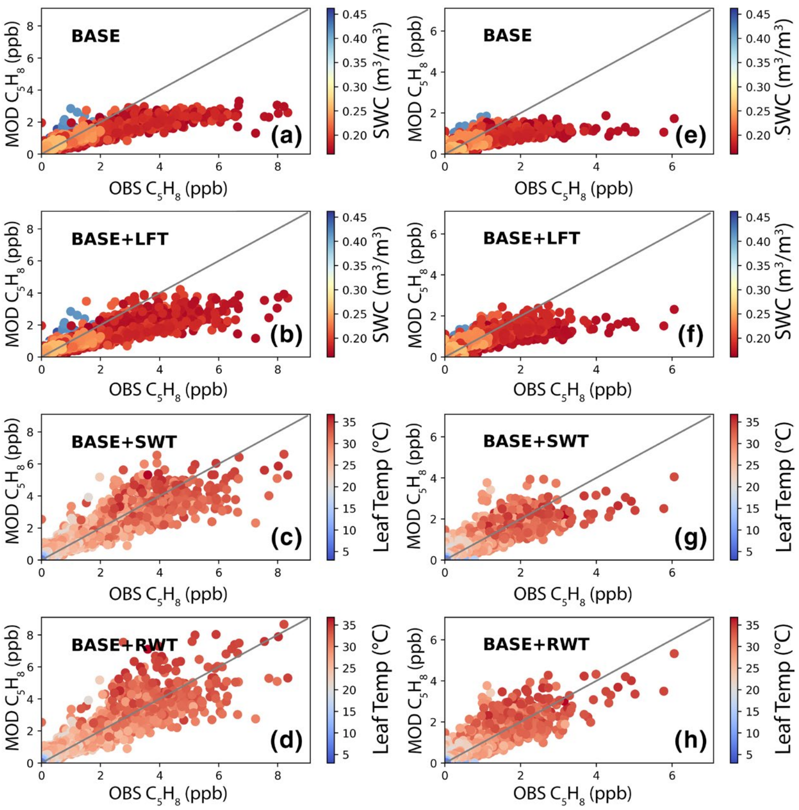

FIGURE 5 Scatter plots of model (MOD) and observed (OBS) isoprene (C_5H_8) mixing ratios for (a and e) BASE coloured by SWC, (b and f) BASE+LFT coloured by SWC, (c and g) BASE+SWT coloured by temperature, (d and h) BASE+RWT coloured by temperature. Panels (a–d) show the top of the canopy (15.6 m) and panels (e–h) the middle of the canopy (13.5 m). Figure S3 in the Supporting Information reproduces these scatter plots for the trunk and near-surface levels

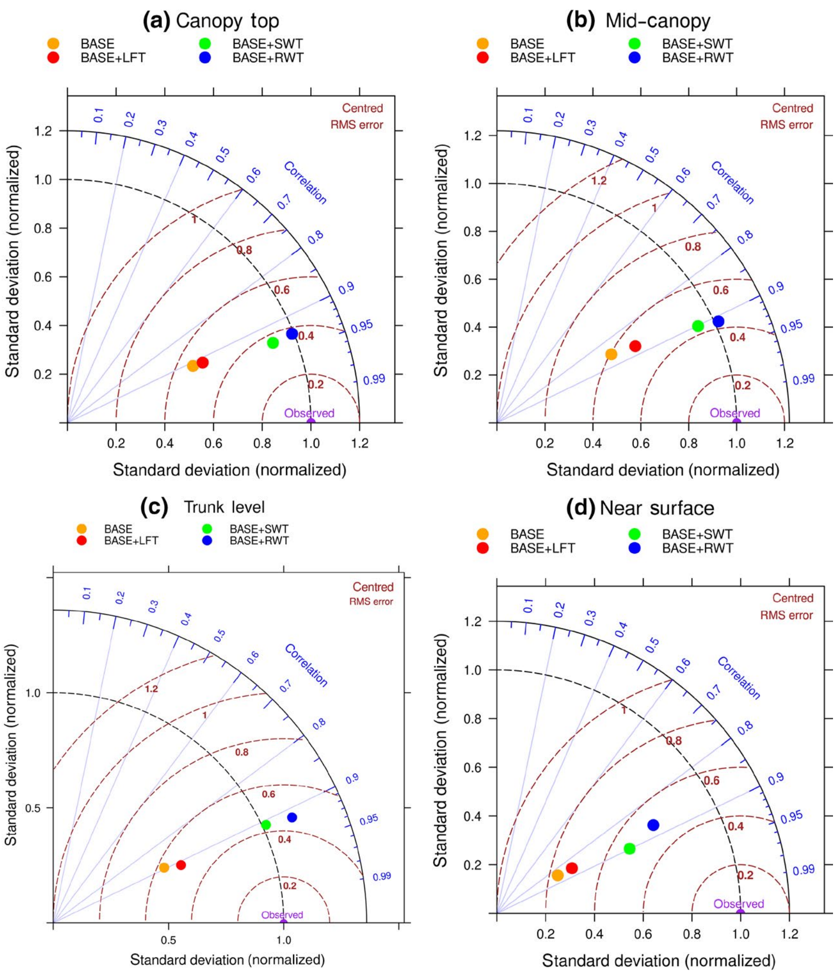

FIGURE 6 Taylor diagram showing model output statistics from the four simulations for (a) top of canopy (15.6 m), (b) middle of canopy (13.5 m), (c) trunk level (7.1 m) and (d) near surface (0.8 m). Dashed black and brown curves and solid blue lines show normalized standard deviation, centred root mean squared error (RMS error) and correlation coefficients, respectively, against observations. The observed isoprene mixing ratios are summarized by the purple circle with a normalized standard deviation of 1.0, RMS error of 0.0 and correlation of 1.0. The summary statistics for the four model simulations are shown by orange (BASE), red (BASE+LFT), green (BASE+SWT) and blue (BASE+RWT) circles. Note the change in scale of standard deviation on panel (c)

shown in Figure 4c,f, further improves the model performance during the heatwave–drought. Mean isoprene mixing ratios during this period increase from 1.87 ppb in BASE+SWT to 1.98 ppb in BASE+RWT, equal to the average of observed values. Figure 5d,h indicates no systematic model bias and the use of a rewetting-enhanced soil moisture activity factor enables the model to capture the higher observed concentrations following rewetting episodes which all previous simulations failed to reproduce. The average isoprene mixing ratio during these rewetting periods is 1.98 ppb compared to 2.05 ppb in the observations, that is, an underestimation of only ~3%. The overall model performance statistics are depicted in Figure 6. While there is no significant difference between the overall correlation and RMSE values in BASE+SWT and BASE+RWT, there is a clear improvement in the model's ability to match the variability shown by the observations with a normalized standard deviation of 0.97 in BASE+RWT compared to 0.89 in BASE+SWT. Compared to BASE, there is ~80% and ~50% improvement in *SD* (0.97 in BASE+RWT vs. 0.61 in BASE) and RMSE (0.41 in BASE+RWT vs. 0.60 in BASE), respectively.

3.4 | Time series of results

Figure 7 shows the isoprene mixing ratios for the period July 22–27 2018, selected as it falls within the heatwave–drought and includes the first of the rainfall events. These plots provide further evidence that all model configurations reproduce the observed diurnal patterns

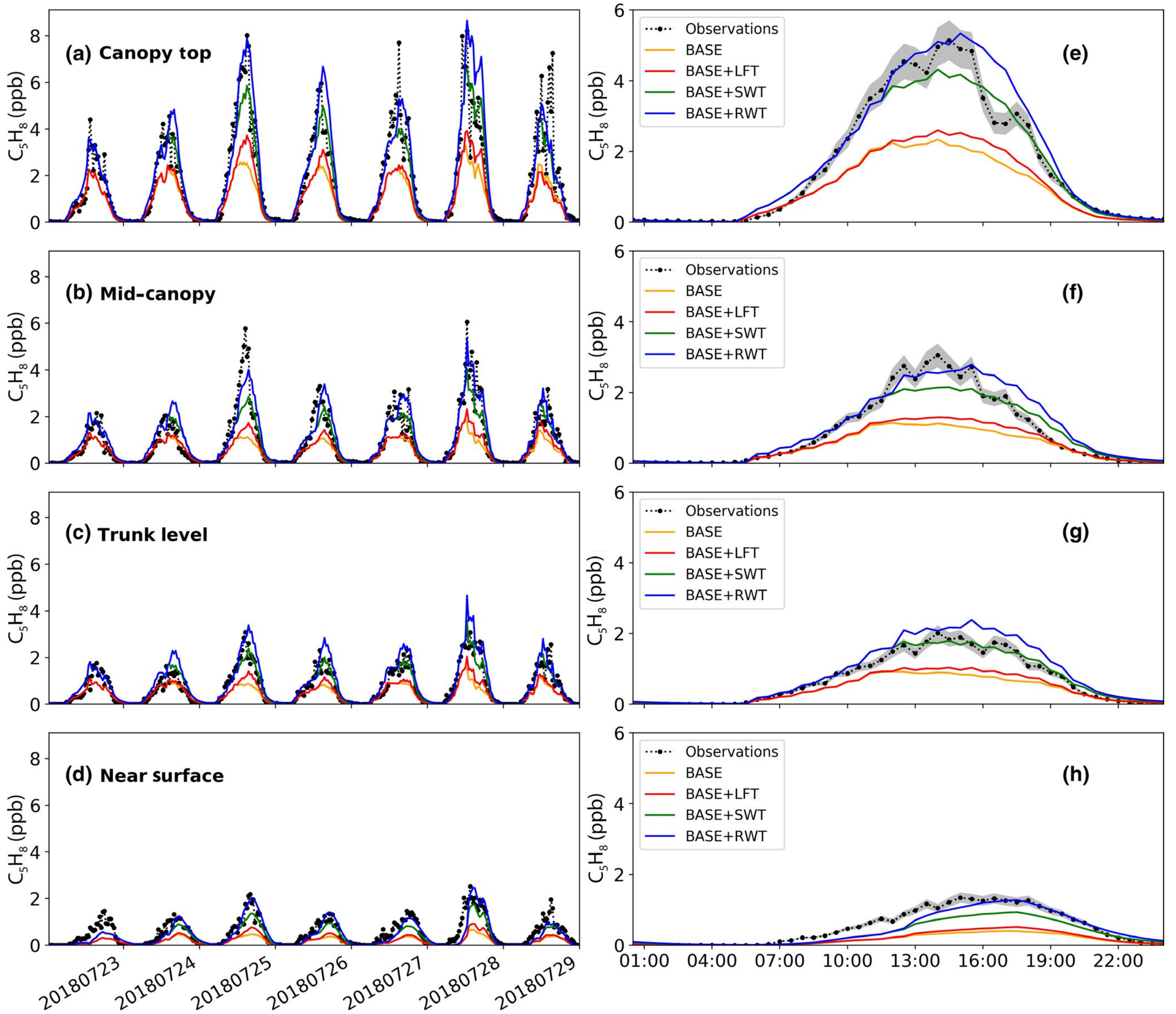

FIGURE 7 (a–d) Time series of isoprene mixing ratios for a selected period during the heatwave–drought (22–27 July 2018) and (e–h) average diurnal profiles of isoprene mixing ratios for the same period. Black dashed lines are observations while the models are coloured orange (BASE), red (BASE+LFT), green (BASE+SWT) and blue (BASE+RWT). The grey shading indicates the uncertainty limits (±11%) around the observations. (a) and (e), (b) and (f), (c) and (g) and (d) and (h) are top of canopy, middle of canopy, trunk and near-surface levels, respectively

of isoprene concentrations at Wytham Woods at the top 3 levels, as expected given the strong dependency of isoprene emissions on temperature and PAR but confirm the earlier results from Figures 2 and 4 that BASE and BASE+LFT models systematically and substantially underestimate isoprene mixing ratios during this period. All three experiments improve model estimations of isoprene concentrations over BASE especially during the middle of the day when observed concentrations peak. Figure 7a–d shows clearly the effect of adding a rewetting-induced enhancement in isoprene emissions (Equation 10). For 22 July, when the rewetting effect is not active, the BASE+SWT and BASE+RWT lines overlap but they diverge between 23 and 27 July following rewetting. Figure 7h shows that all the simulations underestimate observed concentrations near the surface in the early part of the morning (before mid-day), which we ascribe to more light reaching the lower levels in the canopy than is currently accounted for in the model. Figure 7 confirms that BASE+RWT provides the overall best fit when compared to the observations at all levels.

4 | DISCUSSION

Wytham Woods experienced a heatwave and moderate drought (heatwave–drought) during a 7 week period in the summer of 2018 during which time the soil moisture at the site decreased from 0.46 m^3/m^3 (just below field capacity) to 0.16 m^3/m^3 (just above wilting point). Continuous measurements of isoprene mixing ratios were made at the site during the WIsDOM campaign which was conducted in May–October 2018. The aims of our study were to determine how well a 1D canopy exchange model (FORCAsT) could capture the observed changes in isoprene concentrations during the heatwave–drought and to use the model to explore the environmental factors driving these changes. Modelled isoprene mixing ratios did increase substantially during the heatwave–drought in response to large increases in foliage emissions, driven by high temperature and PAR, but not to the extent observed. We conclude that the algorithms currently used in emissions models are unable to account for the actual increase in emission rate under such conditions. We hypothesize that the increase in emission rates during the heatwave–drought was most likely a mechanism to cope with abiotic stress as previously suggested by Holopainen (2004), Loreto and Velikova (2001), Peñuelas and Llusià (2002), Sharkey (1996), and in particular due to low soil moisture.

Many previous studies of the effect of soil water deficit on isoprene emissions have shown a decrease in emission rates with increasing severity of drought (e.g. Pegoraro et al., 2005; Seco et al., 2015) leading to the development of algorithms that decrease the isoprene activity factor (γ_{iso}) in response to decreasing SWC (Guenther et al., 2006). This approach has been used in emission models (e.g. Emmerson et al., 2019; Guenther et al., 2006; Jiang et al., 2018) with good results for severely drought-impacted sites. However, other studies have reported that isoprene emissions are enhanced during periods of mild or moderate drought and Potosnak et al. (2014) demonstrated that the ecosystem-scale response is dependent on drought severity. Some studies have also reported an increase in isoprene after rewetting (e.g. Brilli et al., 2007; Penuelas et al., 2009; Sharkey & Loreto, 1993). The isoprene measurements made during the WIsDOM campaign (Ferracci et al., 2020 in prep) together with the findings from our model simulations support the observation that isoprene emissions can increase under moderate drought conditions and after rewetting resulting in strong enhancements in canopy concentrations. Our model results (Figure S4) also provide evidence in support of the previous observations that isoprene emissions and photosynthesis (often quantified as gross primary production, at an ecosystem scale; e.g. Brilli et al., 2007; Pegoraro et al., 2004) are uncoupled during periods of drought stress.

Emissions models have been shown to perform well in both the unstressed and severe drought phases (e.g. Emmerson et al., 2019; Guenther et al., 2012; Jiang et al., 2019) but underestimate observed concentrations during the mild-to-moderate drought phase (Potosnak et al., 2014; Seco et al., 2015). Conceptual models (Niinemets, 2010; Potosnak et al., 2014) have been developed to explain the impacts of mild droughts on isoprene emissions but these have not been tested until now. We hypothesize that drought severity is the main determinant of changes in isoprene emission rates at the ecosystem scale as well as in the laboratory and that the previous field campaigns used to develop and verify the Guenther soil moisture activity factor (see Pegoraro et al., 2004; Seco et al., 2015) encountered soil water deficits that were more severe than those at Wytham Woods in 2018. Indeed, the Ozark site (described in Gu et al., 2006) which has been used in parameterizing the Guenther soil moisture activity factor experienced two consecutive years of drought in 2011 (mild) and 2012 (severe). 2012 experienced the lowest rainfall in that decade and isoprene emissions decreased significantly (Seco et al., 2015). However, similar to Wytham Woods, isoprene fluxes were observed to increase at the Ozarks during the mild phase of the drought in 2011 (Potosnak et al., 2014).

Potosnak et al. (2014) hypothesized that an increase in leaf temperature due to reductions in transpiration during drought stress is responsible for the increase in isoprene emissions as emission rates depend on leaf rather than air temperature. We found that using a leaf temperature-based isoprene emission activity factor did improve model reproduction of observed isoprene mixing ratios but a substantial underestimation remained. We therefore incorporated a soil moisture activity factor, based on the parameterization of Keenan et al. (2010) for changes in photosynthesis, that increases isoprene emissions under moderate drought conditions, that is, when SWC is close to but slightly above the critical value for the soil at which the standard (severe drought) soil moisture activity factor can be applied. We found that using this new activity factor to account for soil moisture stress when estimating isoprene emission rates improved model reproduction of observed isoprene mixing ratios during the moderate drought without compromising model performance during the rest of the season. However, this was not in itself sufficient to capture the enhancement in isoprene concentrations observed after rainfall events, when soil moisture increased substantially. We found it necessary to further modify our activity factor to account for these episodes, on the hypothesis that these rewetting events were of sufficient intensity to provide near-surface roots access to water, leading to increased foliar activity and isoprene synthesis. Using this soil water and rewetting-based modifying factor that increased isoprene emission rates, a further 30% improved the model fit to observations by 50% based on the root mean squared error. In comparison, Brilli et al. (2007) observed a 20%–60% increase in isoprene emissions from saplings following soil rewetting. These experimental modelling results provide evidence that previous laboratory-based observations of the effect of mild-to-moderate drought stress and soil rewetting on bVOC emissions (e.g. Brilli et al., 2007; Centritto et al., 2011; Loreto & Schnitzler, 2010; Pegoraro et al., 2004) are also observable at the ecosystem scale.

Many field sites do not routinely measure either soil moisture or leaf temperature; our parameterizations are therefore only appropriate for model frameworks with a detailed land surface module. We performed two further experiments using air temperature and vapour pressure deficit (VPD), both readily available data products, as a proxy for the effects of leaf temperature and SWC. VPD, which can be readily calculated from standard meteorological measurements, increases with increasing temperatures and declining soil moisture. Although VPD is not a physiologically robust metric for assessing soil and foliar water availability, we found that an isoprene emission activity factor based on VPD improved modelled isoprene mixing ratios compared to the base case. Our air temperature and VPD parameterization and results are shown in Equations (S1) and (S4), Figures S5–S8 and Table S1. Although not as successful as the rewetting simulations (e.g. there is a ~10% and ~15% improvement on BASE RMSE in BASE+T and BASE+VPD, respectively, compared to ~50% in BASE+RWT), our results show that VPD in particular could be used to improve simulated emissions at sites where soil moisture or leaf temperature measurements are not available and in models without a detailed land surface parameterization.

The Guenther et al.'s (2006, 2012) algorithms reproduce observed isoprene concentrations or fluxes well in unstressed environments and in cases of severe drought. The methods developed in this paper are intended to be used in cases of mild-to-moderate drought which until now has remained a modelling challenge.

Prior to the summer of 2018, Wytham Woods experienced only infrequent moderate-to-severe droughts (in 1976, 1995–1997 and 2003; Mihók, Kenderes, Kirby, Paviour-Smith, & Elbourn, 2009). It is projected that the incidence of droughts in southern England will increase in frequency, duration and severity under future climate change (e.g. Milly, Dunne, & Vecchia, 2005; Schär et al., 2004; Vidale, Lüthi, Wegmann, & Schär, 2007). The summer of 2018 could therefore be viewed as a 'natural experiment' that allowed us to investigate possible future biogenic emissions from Wytham Woods and similar temperate mixed woodlands. We found that the emissions algorithms currently included in global emissions and chemistry-climate models underestimated total isoprene emissions during the heatwave–drought by ~40% and by ~20% over the entire June–September period. While the findings of this single experiment should not be extrapolated to a global scale, if these are representative of the wider picture, the magnitude of the modelled change in emissions would have a major impact on local- to regional-scale emissions and hence atmospheric chemistry and composition in many world regions.

The main advantage of our natural experiment is that we were able to observe the impacts on mature trees in a real-world (uncontrolled) environment. Such conditions are impossible to reproduce in laboratory-based experiments that investigate potential impacts of global climate change on tree physiology and bVOC emissions. Saplings and young plants, the preferred options in laboratory experiments, do provide useful information about the general behaviour of trees under various environmental stressors, but cannot replicate the combinatorial stresses and symbioses experienced by mature trees and full ecosystems. The results from WIsDOM and previous measurement campaigns carried out on mature trees (e.g. Genard-Zielinski et al., 2018; Llusia et al., 2016; Potosnak et al., 2014) show that emissions characteristics under heatwave–droughts in the natural environment differ from those observed in many laboratory experiments. However, it can be expected for the response to be dependent on tree species, with some adapted to withstand periods of water limitation, and on soil properties. It is clear therefore that more ecosystem-scale observations are required under mild, moderate and severe drought conditions if we are to understand how future changes in precipitation and ground-water levels are to affect isoprene emissions.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

AUTHOR CONTRIBUTIONS

All authors designed the experiment and contributed to writing the manuscript. F. Otu-Larbi and K. Ashworth carried out the modelling work and analysed the output data. C. Bolas, V. Ferracci and Z. Staniaszek collected and processed the observational data from Wytham.

DATA AVAILABILITY STATEMENT

FORCAsT 1.0 and the data used in this study are available by request to the corresponding authors.

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section.

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