

This discussion paper is/has been under review for the journal Atmospheric Chemistry and Physics (ACP). Please refer to the corresponding final paper in ACP if available.

Identification and quantification of gaseous organic compounds emitted from biomass burning using two-dimensional gas chromatography/time-of-flight mass spectrometry

L. E. Hatch¹, W. Luo¹, J. F. Pankow¹, R. J. Yokelson², C. E. Stockwell², and K. C. Barsanti¹

¹Department of Civil and Environmental Engineering, Portland State University, Portland, Oregon

²Department of Chemistry, University of Montana, Missoula, Montana

Received: 15 August 2014 – Accepted: 19 August 2014 – Published: 10 September 2014

Correspondence to: K. C. Barsanti (barsanti@pdx.edu)

Published by Copernicus Publications on behalf of the European Geosciences Union.

23237

Abstract

The current understanding of secondary organic aerosol (SOA) formation within biomass burning (BB) plumes is limited by the incomplete identification and quantification of the non-methane organic compounds (NMOCs) emitted from such fires. Gaseous organic compounds were collected on sorbent cartridges during laboratory burns as part of the fourth Fire Lab at Missoula Experiment (FLAME-4), with analysis by two-dimensional gas chromatography/time-of-flight mass spectrometry (GC × GC/TOFMS). The sensitivity and resolving power of GC × GC/TOFMS allowed the acquisition of the most extensive data set of BB NMOCs to date, with measurements for 722 positively or tentatively identified compounds. Estimated emission factors (EFs) are presented for these compounds for burns of six different vegetative fuels, including conifer branches, grasses, agricultural residue, and peat. The number of compounds detected from individual burns ranged from 129 to 474, and included extensive isomer groups. For example, 38 monoterpene isomers were observed in the emissions from coniferous fuels; the isomeric ratios were found to be consistent with those reported in relevant essential oils, suggesting that the composition of such oils may be very useful when predicting fuel-dependent terpene emissions. Further, eleven sesquiterpenes were detected and tentatively identified, providing the first reported speciation of sesquiterpenes in gas-phase BB emissions. The calculated EFs for all measured compounds are compared and discussed in the context of potential SOA formation.

1 Introduction

Biomass burning (BB) emissions can strongly influence tropospheric chemistry and climate. Wildfires and prescribed burns occur under conditions and with biomass fuel types that vary greatly. Fires emit high concentrations of particulate matter (PM) and gases; such gases include nitrogen oxides (NO_x), carbon dioxide/monoxide, and non-

23238

methane organic compounds (NMOCs) of varying volatilities. During plume evolution, these emissions may react photochemically to form secondary pollutants (e.g., ozone) (Crutzen and Andreae, 1990). The primary emissions and secondary species affect human health and climate. Atmospheric PM is associated with negative health effects, such as cardiovascular and respiratory diseases (Poschl, 2005). Further, long-range transport of BB emissions can carry species 1000+ km from a fire source (Crutzen and Andreae, 1990), thereby extending the health and environmental consequences of smoke well beyond fire-prone regions; for example, emissions from wildfires occurring in Russia have impacted the Arctic (Wang et al., 2011).

BB particles can influence the radiative balance of the atmosphere directly by scattering or absorbing solar radiation (Hobbs et al., 1997), and indirectly by acting as cloud condensation nuclei (CCN) (Desalmand and Serpolay, 1985; Reid et al., 2005) and ice nuclei (IN) (Petters et al., 2009). A large number of BB particles in a forming cloud can increase the number of CCN yielding smaller cloud droplets, thereby increasing cloud albedo (Crutzen and Andreae, 1990). This effect may alter precipitation patterns and thus the hydrological cycle (Lohmann and Feichter, 2005; Andreae et al., 2004).

BB is the second largest global source of NMOCs; these species may undergo photochemical processing ("aging"), leading to lower volatility or more soluble compounds that can condense into existing particles and form secondary organic aerosol (SOA) (Kroll and Seinfeld, 2008; Hallquist et al., 2009). Laboratory and field studies have shown a wide range of organic aerosol (OA) mass enhancement ratios (< 1 to 4) following aging of BB smoke (Grieshop et al., 2009; Hennigan et al., 2011; Ortega et al., 2013; Jolleys et al., 2012; Yokelson et al., 2009; Akagi et al., 2012; Wigder et al., 2013; Vakkari et al., 2014), demonstrating high variability in BB emissions and/or plume chemistry. Further, Hennigan et al. (2011) reported extensive oxidation of BB primary OA (POA) during laboratory aging experiments, suggesting that physicochemical properties of OA may change regardless of net loss or production of OA mass. Highly oxidized SOA and aged POA components can influence particle hygroscopicity

23239

(Saxena et al., 1995) and CCN activity, thereby exacerbating the effects of BB-derived particles on biogeochemical cycles and planetary albedo.

Efforts toward understanding SOA formation in BB plumes have been hindered by limited identification and quantification of the NMOCs emitted by fires (Akagi et al., 2011). In a recent study using data from open-path Fourier transform infrared spectroscopy, proton-transfer-reaction ion-trap mass spectrometry, and gas chromatography/mass spectrometry (GC/MS), only ~ 50–70 % of measured gas-phase organic mass was identified (Warneke et al., 2011; Yokelson et al., 2013), with the majority of the remaining mass likely having lower volatility than the NMOCs routinely measured in BB studies. Thus there is a significant need to better characterize NMOCs in BB smoke. Further, studies have demonstrated that known SOA precursors alone cannot explain observed OA growth in aged BB smoke (Grieshop et al., 2009; Ortega et al., 2013). Given the potentially significant production of SOA from BB, improved measurements of gas-phase SOA precursors within smoke plumes are essential for better assessing the health and climate impacts of BB particles.

Whereas traditional one-dimensional (1-D) GC/MS has been extensively applied toward the characterization of BB emissions (Christian et al., 2004; Simpson et al., 2011; Ciccioli et al., 2001), GC × GC has seen limited application in this field (Ma et al., 2010; Ma and Hays, 2008; Nara et al., 2006). GC × GC employs two columns to extend the separation capabilities allowed by 1-D GC. Typically, a non-polar column is utilized for the primary separation based on volatility; slices of the analyte flow are directed to a second column for separation according to polarity or polarizability (Beens et al., 1998). Several characteristics (Mondello et al., 2008) of GC × GC/TOFMS make it a powerful tool for characterizing the highly complex gas-phase components of smoke. These are: (1) high resolving power provides enhanced chromatographic separation, (2) thermal modulation at the interface of the primary and secondary columns refocuses eluting peaks leading to significant improvements in signal-to-noise ratio and thus sensitivity, (3) high TOFMS spectral collection rate allows up to 500 full mass spectra (m/z 34–500) to be obtained for a given peak eluting from the secondary column

23240

(the time evolution of the mass spectra can help deconvolute co-eluting compounds), and (4) distinct compound classes form patterns in the 2-D retention space aiding in compound classification. Herein, the first application of GC × GC to broadly characterize the gas-phase emissions of BB is described, including comparisons among the emissions from burns of selected conifer, grass, crop residue, and peat fuel types.

2 Experimental

2.1 FLAME-4 sampling

Samples were collected during the fourth Fire Lab at Missoula Experiment (FLAME-4) from 3–12 November 2012 in Missoula, Montana. An overview of FLAME-4 has been provided by Stockwell et al. (2014). Controlled burns were conducted in the combustion laboratory of the US Forest Service Fire Science Laboratory (FSL) using a variety of vegetative fuels. The combustion laboratory is described in detail elsewhere (Christian et al., 2004). In these “room burn” experiments, smoke was allowed to mix throughout the FSL combustion chamber (12.5 m × 12.5 m × 22 m); the smoke contained a mixture of emissions from flaming and smoldering combustion. Prior to ignition, each fuel sample was arranged to promote burning under field-relevant conditions (e.g., grasses were standing upright instead of piled). Emissions were sampled from fires of six different globally relevant fuels: black spruce (BS), ponderosa pine (PP), wiregrass (WG), giant cutgrass (CG), Chinese rice straw (RS), and Indonesian peat (IP).

2.1.1 Fuel selection

Black spruce (*Picea mariana*) and ponderosa pine (*Pinus ponderosa*) are coniferous trees native to North America. Black spruce is common throughout many fire-prone ecosystems in the Boreal forest of Canada and Alaska (Cumming, 2001). The BS sample was obtained near Fairbanks, Alaska. Ponderosa pine forests are common throughout the western US/Canada and experience extensive prescribed burning and

23241

wildfire activity (e.g., Veblen et al., 2000). The PP sample was obtained locally in Missoula, Montana. Woody material and needles were burned in the FLAME-4 fires.

Both grassland fuels analyzed – giant cutgrass (*Zizaniopsis miliacea*) and wiregrass (*Aristida stricta*) – predominantly grow in the southeastern US. Prescribed burning is common throughout the SE US as a means of hazard reduction and reforestation (Haines and Busby, 2001). Although CG typically grows in fresh or brackish marshes, these grasslands are still susceptible to burning and prescribed fires are often used within these ecosystems (Wade et al., 2000). Wiregrass is a bunchgrass commonly associated with longleaf pine forest ecosystems throughout the southern coastal plains. These ecosystems have been shown to benefit from frequent prescribed burning (Brockway and Lewis, 1997).

Rice straw (*Oryza sativa*) is an agricultural waste product commonly burned throughout Asia to clear fields. The RS sample was obtained from China, where the majority of BB has been attributed to crop residue (Streets et al., 2003). A peat sample was also imported from Indonesia, where 80 % of the peatlands in Southeast Asia are located (Chang and Song, 2010). Extensive deforestation and drainage of peatlands throughout Indonesia have greatly increased the susceptibility of peat to fire activity (Heil, 2007). Because peat deposits can be very deep and may smolder for months at a time (Heil, 2007), peat fires can be a major source of pollution to the atmosphere (Page et al., 2002).

2.1.2 ATD cartridge samples

Adsorption/thermal desorption (ATD) cartridges were used to collect gaseous NMOCs. The cartridges were 8.9 cm long × 0.64 cm o.d. stainless steel tubes with an inert, internal SilcoTek coating; each contained a dual-sorbent bed composed of 100 mg Tenax TA 35/60 and 200 mg Carbograph 1 TD 60/80 in series (Camsco, Inc., Houston, TX). The use of multiple sorbents permits compounds with a wide range of volatilities to be collected (Pankow et al., 2012). Prior to shipment to the field, each cartridge was conditioned at ~ 290 °C for 1 h with a continuous flow of precleaned helium (~ 250 mL min⁻¹).

23242

A glass-fiber filter coated with sodium thiosulfate was placed upstream of the cartridge in the sampling train to prevent particles and ozone from reaching the sorbent (Helmig, 1997). In separate tests, these filters were found to scrub ozone at ~ 760 ppb with greater than 90 % efficiency from ~ 3 L sample volume and were thus considered sufficient for removing the negligible ozone expected in fresh BB smoke (Akagi et al., 2013). A new filter was used with each sample. The filter holder, sampling line, and all fittings were Teflon. Some adsorption of semi-volatile compounds to the tubing and filter may have occurred, though no corrections were applied. Background samples were taken shortly before fire ignition. Smoke samples were collected after the smoke had equilibrated throughout the burn chamber. Breakthrough tests were conducted wherein two cartridges were placed in series to determine which compounds were incompletely trapped on a single cartridge. All sample volumes were ~ 2 L, with collection taking place over 15 min at a flow rate of ~ 150 mL min⁻¹. After sampling, the ATD cartridges were sealed with compression fittings using Teflon ferrules, and stored at < 0 °C. The samples were analyzed within 1 month of sampling.

2.1.3 Filter-desorption samples

To further characterize the volatilizable NMOCs that were not detected in the gas-phase cartridge samples, PM samples were collected on glass-fiber filters (0.7 μ m pore size, ~ 8 L min⁻¹, ~ 60 min). Prior to shipment to the field, the glass-fiber filters were baked at ~ 130 °C for ~ 8 h. Following sample collection, the filters were immediately packaged in pre-baked aluminum foil and stored at < 0 °C for up to one day prior to desorption. Volatilizable NMOCs were desorbed by passing clean N₂ through the filter (150 mL min⁻¹) at room temperature and trapped on an ATD cartridge. The clean N₂ source was supplied by scrubbing laboratory-grade N₂ with two ATD cartridges in series. Comparison of the data from the second scrubber cartridges with those from blank cartridges indicated that the contaminants in the N₂ carrier gas were effectively removed. As separate quality control tests, a blank filter and a background PM sample (collected in the burn chamber prior to ignition) were treated by the same desorption

23243

method. The mass of the background filter before and after PM collection indicated that adsorbed species volatilized from the filter during sampling. Therefore the results from the BB filter desorption samples were not quantified due to uncertainties in the masses of collected PM. We report only the compounds identified from the filters that were not detected in the cartridge samples (with the exception of $\geq C_{14}$ hydrocarbons because they were detected in only one cartridge sample).

2.2 Chemical standards

Calibration curves were determined for ~ 275 standard compounds in order to positively identify and quantify these components (listed in boldface in Table A1). Standards were prepared from (1) a commercial mixture (PIANO mix, Sigma Aldrich, St. Louis, MO) containing ~ 140 compounds (alkanes, alkenes, and aromatic hydrocarbons) that was injected (5.0 μ L) into a pre-cleaned and purged 2 L glass reservoir to produce a gas-phase standard, and (2) individual compounds dissolved in methanol. Seven standards (concentration levels) each were made from the PIANO mix and methanol solution. Each standard was injected onto an ATD cartridge and carried into the sorbent bed by a flow (~ 50 – 75 mL min⁻¹) of precleaned helium.

Initial analyses of the PIANO standards indicated that alkanes $> C_{10}$ remained partially adsorbed to the walls of the glass reservoir. To determine appropriate corrections, the PIANO standards were analyzed using a GC \times GC instrument with flame ionization detection (FID). Because mass-based FID response factors (RF, area counts ng⁻¹) are approximately independent of carbon number (Tong and Karasek, 1984), the GC \times GC/FID data were used to estimate the mass percentage present in the gas phase at the time of cartridge spiking for each of the $> C_{10}$ alkanes by comparison to the average RF measured for C₇–C₉ alkanes. The measured gas-phase percentages ranged from ~ 96 % for decane to ~ 33 % for pentadecane. The adjusted mass amounts were used in the GC \times GC/TOFMS calibration curves.

2.3 ATD cartridge analyses

Samples and standards were analyzed using a Pegasus 4D GC × GC/TOFMS (Leco Corp., St. Joseph, MI). Each ATD cartridge was desorbed using an ATD 400 system (Perkin-Elmer, Waltham, MA) connected to the GC × GC injection port via a fused silica transfer line at 225 °C. The flow direction through the cartridge during desorption was the reverse of that for sampling to prevent lower volatility analytes from contacting the Carbograph sorbent. Each cartridge was desorbed (285 °C, 10 min, 40 mL min⁻¹) onto a Tenax focusing trap (−20 °C). That trap was then desorbed (300 °C, 3 min) to transfer the analytes to the GC × GC injection port. The injection split ratio was 10 : 1. The GC × GC conditions are summarized in Table 1.

Samples were processed using the ChromaTof software package (Leco Corp., St. Joseph, MI). A peak was discarded if its area was < 200 000 units or if the mass spectral match similarity relative to the NIST mass spectral database was < 750 (out of 1000). The concentration of each compound measured in the corresponding background sample was subtracted from the amount found in the smoke sample. For the ponderosa pine and Indonesian peat smoke samples, background samples were unavailable; the background measurements for the other four samples were averaged and applied instead. Standard deviations were applied as the uncertainty in the average background concentrations; among the four background samples, concentrations varied ~ 10–160 % of the average. Chromatographic peaks were removed from consideration if they did not survive background subtraction or were not statistically different from zero after background subtraction.

Cases of ambiguous isomer assignments (because an authentic standard had not been used) were based whenever possible on published retention indices (e.g., Sojak et al., 1984, 1973; Stein, 2013). Otherwise, peaks were characterized here solely by chemical formula as assigned by the best mass spectral match(es).

Each positively identified compound (i.e., standard available) was quantified using calibration curves; tentatively identified analytes were quantified using the calibration

23245

curve of the most chemically similar standard compound. With a few exceptions (noted below), all components were calibrated using the deconvoluted total ion current. For analytes whose peak areas were low relative to the y-intercept of the calibration regression line, it was necessary to use RFs (area counts ng⁻¹) instead. Generally, the average RF of the three lowest concentration standards was used. Error bars were calculated from the standard error in the linear regression of the calibration curve or the standard deviation of the average RF. The uncertainty for positively (tentatively) identified compounds was set to a minimum of 20 % (50 %). Mixing ratios used in determining emission factors (see Sect. 3.2) were calculated using the ambient temperature and pressure measured in the burn chamber. For the benzene and toluene peaks in some cartridge samples, the MS detector was saturated for the major ions in the mass spectra; thus these compounds were quantified using a minor ion. The same approach was required for camphene in the black spruce cartridge sample. The reported values for these species likely reflect lower limits.

3 Results and discussion

3.1 Scope of the GC × GC data

The GC × GC/TOFMS chromatograms of the cartridge samples from the six burns are shown in Figs. 1–6; the compounds detected are listed in Table A1. The data have been organized into major chemical classes (panel b of Figs. 1–6 and Table A1). For reference, an example chromatogram highlighting regions of the major chemical classes is included in the Supplement. Compounds with a wide range of volatilities and functionality were detected, from C₃ polar compounds through C₁₅ hydrocarbons (Table A1). The range of detectable compounds was limited by the cartridge sampling and analysis conditions.

Lower volatility compounds were not well characterized by this approach. Such compounds may be adsorbed by the filter used upstream of the sampling cartridge to re-

23246

move particles and ozone. Additionally, highly polar gases are not amenable to analysis by GC. For instance, analysis of standards demonstrated that hydroxy phenols (e.g., resorcinol) did not elute from the column set used for this work. Further, with the Stabilwax secondary column utilized, several polar compounds (e.g., phenols and furfural) “wrapped-around” (i.e., did not elute within one modulation period). Such peaks are thus very broad in the second dimension and may also appear in regions of the chromatogram typical of significantly less polar compounds. These features are most pronounced for the RS sample (Fig. 5), which contained the highest fraction of oxygenated compounds.

On the high end of the volatility range, we have omitted all compounds eluting before 3-methyl-1-butene, the earliest eluting C₅ hydrocarbon (HC). HCs ≤ C₃ were not trapped by the Tenax/Carbograph cartridges. Although C₄ HCs were detected, they displayed high breakthrough; the lightest standard (C₅) HC compounds exhibited minimal breakthrough and thus could not be used to quantify the observed C₄ compounds. Light (≤ C₄) HCs have been previously shown to dominate the overall HC emissions from BB (e.g., Schauer et al., 2001; Akagi et al., 2011), however these components have been generally well characterized by other methods (e.g., canister samples (Simpson et al., 2011)) and typically are not significant precursors to atmospheric SOA (Seinfeld and Pankow, 2003).

Although several reported oxygenated compounds displayed high breakthrough as well, appropriate standard compounds allowed reasonable quantification. For such compounds, the corresponding standards showed evidence of breakthrough based on the GC × GC/FID data; thus application of the calibration curve somewhat corrects for the low trapping efficiency. However, comparison with co-located measurements (not shown) indicates that our measured concentrations of acetone and acetonitrile were comparatively low and therefore values reported here should be considered a lower limit. The same may be true of acrolein, although quantified co-located measurements were not available to verify the results. Furan also displayed very poor trapping efficiency in the samples and standards. However, tests showed that the breakthrough

23247

was quite consistent and application of the calibration curves yielded results in good agreement with co-located measurements; thus we expect the reported values of furan to be accurate.

3.2 Emission factors

Emission factors (EF, g kg⁻¹ of dry fuel burned) were calculated by the carbon mass balance method (Yokelson et al., 1999; Stockwell et al., 2014):

$$EF_X = F_C \times \frac{MM_X}{MM_C} \times \frac{\frac{\Delta X}{\Delta CO_2}}{\sum_i^n \left(NC_i \times \frac{\Delta Y_i}{\Delta CO_2} \right)}. \quad (1)$$

F_C is the mass fraction (g kg⁻¹) of carbon in the dry fuel and was measured by an independent laboratory for each fuel (Table A1). MM_X and MM_C are the molar masses of compound X and carbon, respectively. ΔX is the background-subtracted (“excess”) mixing ratio of compound X; $\Delta X/\Delta CO_2$ (or $\Delta Y/\Delta CO_2$) is the emission ratio (ER) of compound X (or Y) relative to CO₂ (ERs are also commonly referenced to CO for smoldering compounds). NC_i is the number of carbon atoms in compound Y_i . The summation represents the total carbon emitted during combustion, assuming complete volatilization; it includes CO₂, CO, and C_{1–3} alkanes/alkenes, as measured by open-path Fourier-transform infrared spectroscopy (OP-FTIR) (Stockwell et al., 2014) and averaged over the corresponding cartridge sampling periods. Strictly speaking, the summation should also include minor NMOCs and particulate carbon, however ignoring these components introduces errors on the order of only a few percent (Yokelson et al., 2013), which is well within the reported uncertainties.

The fire-integrated modified combustion efficiency (MCE, $\Delta CO_2/(\Delta CO_2 + \Delta CO)$) for the six burns are included in Table A1. MCE is a measure of the relative contributions of flaming and smoldering combustion (Yokelson et al., 1996). Higher values (approaching 0.99) are indicative of pure flaming combustion, whereas lower values (~ 0.8) in-

23248

dicating pure smoldering combustion. Intermediate values reflect a mix of flaming and smoldering combustion.

MCEs and EFs for the PP and BS burns were compared to those presented by Yokelson et al. (2013) for coniferous canopy fires. The MCEs in this work (PP, 0.927 and BS, 0.933) are similar to that reported by (Yokelson et al., 2013) (0.925 ± 0.036). In a correlation plot, the EFs for 48 overlapping compounds (Fig. 7) are scattered about the 1 : 1 line, demonstrating that there was no systematic difference in these laboratory measurements relative to Yokelson et al. (2013). Of the disparate points, several reflect monoterpene isomers, whose emissions can vary significantly among different plant species (see Sect. 3.3.5).

The MCE of the IP burn in this work (0.832) was nearly identical to a laboratory IP burn of Christian et al. (2003) (0.838). However, the calculated EFs for IP smoke (Table A1) are ~ 2 – 7 -fold lower than those reported by Christian et al. (2003) for the 6 overlapping compounds. For comparison, the EFs based on OP-FTIR measurements for the FLAME-4 IP burns (Stockwell et al., 2014) averaged ~ 9 -fold lower to ~ 3 -fold higher than those by Christian et al. (2003). The differences in measured EFs likely arise from the different peat samples: the FLAME-4 peat sample was obtained from a previously burned/logged peat forest in Kalimantan, whereas the peat burned by Christian et al. (2003) came from Sumatra. Given the wide variability in reported EFs, additional measurements of Indonesian peat fire emissions should be undertaken to help constrain their EFs. Christian et al. (2003) have also reported emissions from Indonesian RS. The MCE during their burn (0.811) was much lower than that of the Chinese RS fire measured in this study (0.942); thus the emissions of smoldering compounds were significantly higher in the Christian et al. (2003) study. The different combustion conditions were largely due to the fuel orientations. In the study by Christian et al. (2003), RS was burned in a dense pile, as often occurs in non-mechanized agriculture. The FLAME-4 RS sample was burned as unpiled field residue, for which a similar MCE of ~ 0.93 has been measured for RS under ambient burn conditions

23249

(Oanh et al., 2011). The relative importance of these two orientations is not well known (Akagi et al., 2011).

For the WG and CG fires, there are no available emission measurements for compounds that can be compared with our data.

3.3 NMOC observations

Including NMOC emissions from all six burns, a total of 688 compounds were positively or tentatively identified in the gas-phase cartridge samples (Table A1) and a further 34 compounds were identified solely in the filter-desorption samples (Table 2). Of these compounds, ~ 30 – 50 % were positively identified across the six burns. There was significant variation in the number of compounds detected in each smoke sample, ranging from 129 (WG) to 474 (PP) (Table A1). The grass fires produced the fewest compounds, as well as the lowest overall NMOC emissions, with total EFs of 1.42 and 1.08 g kg^{-1} for CG and WG, respectively, compared to 3.36 – 14.57 g kg^{-1} for the other fuels (Table A1). The lower emissions cannot be explained entirely by differences in combustion efficiency because the MCE of the CG fire was similar to those from the coniferous fuels, which displayed ~ 6 – 8 -fold higher total EF (Table A1).

Abundant isomers were present in nearly all chemical classes, for example: 17 $\text{C}_{10}\text{H}_{14}$ isomers (aromatic HCs), 31 C_7H_{12} isomers (aliphatic HCs), 38 $\text{C}_{10}\text{H}_{16}$ isomers (monoterpenes), and 13 $\text{C}_5\text{H}_8\text{O}$ isomers (aldehydes and ketones) were detected. Because chemical structure significantly influences chemical reactivity (Ziemann and Atkinson, 2012), it is advantageous to speciate the compounds in these groups to better predict BB plume chemistry. Although in many cases specific structures could not be assigned, future availability of additional standard compounds will enable more thorough chemical identification.

Of the 688 compounds detected, only 75 compounds were present in all 6 cartridge samples (Fig. 8). Most of these were “major” compounds, defined as $\text{EF} > 0.01 \text{ g kg}^{-1}$ in any sample (e.g., benzene, toluene, and furan). These major compounds accounted for 55–81 % of the total EF from the burns. Efforts aimed at improving the representa-

23250

tion of BB SOA in atmospheric models might begin with this group. Of the 242 compounds unique to a single burn, most were present at low levels ("minor", Fig. 8). Aliphatic HCs constituted approximately half of these minor compounds, due to the large number of potential isomers.

5 To more clearly show the relative proportions of the identified compounds, the data were sorted into groups based on functionality and carbon number (b panels, Figs. 1–6). Because these figures do not include compounds that were not well characterized by our approach (e.g., low molecular weight compounds known to have high emis-
10 sions), they do not provide a full accounting of the NMOC emissions. A complete synthesis of the NMOC measurements during FLAME-4 is underway and will be presented in a separate study. Interesting features of each class elucidated by GC × GC/TOFMS, particularly as relevant for SOA formation, are described in the following sections.

3.3.1 Aromatic hydrocarbons

Aromatic HCs represented a major fraction of emissions from all fuels (Figs. 1–6), ex-
15 cept WG (only ~ 10 %, Fig. 4); for CG in particular, aromatic HCs were overwhelmingly dominant (~ 43 %, Fig. 3). The majority of the aromatic emissions were alkyl aromatic HCs, in terms of both EF and number of compounds (Table A1), although significant levels of compounds with unsaturated substituents (e.g., styrene, phenylacetylene, and their substituted analogs) were also detected in the BS, PP, and CG burn emissions
20 (Figs. 1b–3b). In all cases, the most abundant aromatic HC was benzene, followed by toluene, despite being under-predicted by our measurements; this is consistent with prior measurements of aromatic HCs in BB emissions (Akagi et al., 2011; Andreae and Merlet, 2001; Yokelson et al., 2013). Further, higher molecular weight aromatic HCs were detected than are usually reported in gas-phase BB emissions. Many
25 compilations report $\leq C_9$ aromatic HCs (e.g., propylbenzene isomers) (Akagi et al., 2011; Andreae and Merlet, 2001); recently, Yokelson et al. (2013) reported unspeci- ated C_{11} alkyl aromatics. In this work, a number of C_{11} isomers with substituents of varying double bond equivalents (DBE) (0–2) were detected (Table A1) and in the
23251

filter-desorption tests, benzene derivatives as large as nonyl benzene were observed (Table 2). Naphthalene and several methyl naphthalenes, as well as related compounds such as biphenyl and acenaphthylene, were detected in the emissions from all fuels.. Higher molecular weight naphthalene derivatives and polycyclic aromatic HCs (PAHs)
5 were tentatively identified in the filter-desorption samples, including a trimethyl naphthalene isomer and phenanthrene (Table 2).

The chemical structure of aromatic HCs may influence the kinetics and thermody-
namics of SOA formation and will vary from plume to plume depending on the iso-
meric ratios. The atmospheric reactivity of aromatic HCs is dominated by OH addition,
10 for which the reaction rate increases with the number of alkyl substituents and is fur-
ther influenced by their position (Ziemann and Atkinson, 2012 and references therein). For instance, the rate constant of 1,3,5-trimethyl benzene is ~ 10× faster than that of *n*-propyl benzene (Finlayson-Pitts and Pitts, 2000). However, similar SOA yields of ~ 30 % (roughly independent of particle mass concentration) have been measured by
15 Ng et al. (2007) for benzene, toluene, and *m*-xylene under low NO_x conditions (signifi-
cantly lower yields were observed under high NO_x conditions and varied as a function of particle mass concentration). Naphthalene and its derivatives exhibit notably higher SOA yields than the substituted benzenes: up to ~ 73 % under low NO_x conditions and ~ 20–30 % under high NO_x conditions (Chan et al., 2009). Because naphthalene and
20 its derivatives composed up to 17 % (CG) of total aromatic HCs, such compounds may be significant contributors to SOA mass in BB plumes (Chan et al., 2009).

3.3.2 Oxygenated aromatic compounds

Oxygenated aromatic compounds constituted between 3.8 % (BS) to 17 % (CG) of the total EF measured from each fuel. Phenol was the most abundant oxygenated aromatic species emitted for all of the fuels tested (Table A1). Several substituted phenols
25 were also identified, including methyl and dimethyl phenols. Phenolic compounds arise from the pyrolysis of lignin, an amorphous polyphenolic polymer. Guaiacol was the only methoxy phenol detected in the cartridge samples (Table A1); however, several
23252

guaiacol derivatives were volatilized from the filter samples, primarily from the coniferous fuels (Table 2). Conifers are softwoods, which contain lignins composed primarily of guaiacyl units (Shafizadeh, 1982); therefore the presence of many guaiacols is to be expected from such fuels (Jiang et al., 2010; Saiz-Jimenez and De Leeuw, 1986). Several other non-phenolic oxygen-containing aromatic compounds were observed, including furans, aldehydes, ketones, and ethers (Table A1). Little information exists regarding the formation of such compounds in fires, although several have been previously observed in BB smoke (Yokelson et al., 2013; Andreae and Merlet, 2001).

Phenol, alkyl phenols, and guaiacol have been shown to produce SOA in relatively high yields (~ 25–50 %) from OH-initiated gas-phase chemistry (Yee et al., 2013; Nakao et al., 2011). Recently, Smith et al. (2014) observed nearly 100 % SOA yield from the aqueous-phase reaction of phenols with excited state organic compounds. Given the dominance of phenols among the oxygenated aromatic compounds (Figs. 1–6) and their reportedly high SOA yields, phenols are likely to be the most significant SOA precursors in this category. SOA formation from the less abundant oxygenated aromatic compounds (aldehydes, ketone, furans) has not been well characterized. However, benzaldehyde, acetophenone, and benzofuran (including its methyl derivatives) were present in the smoke from all six burns; thus these compounds may be good subjects for future smog chamber studies.

3.3.3 Aliphatic hydrocarbons

Approximately half of all detected compounds were aliphatic HCs, with 0–4 DBE. Up to 33 % (IP) by EF of the aliphatic HC category is attributed to compounds larger than the $\leq C_8$ compounds typically reported in BB emissions (Akagi et al., 2011; Andreae and Merlet, 2001). Few BB studies have measured $> C_9$ aliphatic HCs. Ciccioli et al. (2001) detected up to C_{13} alkanes/alkenes from flaming and smoldering pine wood; Schauer et al. (2001) measured C_{1-9} and C_{18-24} alkanes in the gaseous emissions from pine wood burning, but they do not report the intermediate species. In four of the six FLAME-4 filter-desorption samples, tetradecane and pentadecane were observed (Table 2),

23253

suggesting that intermediate volatility compounds are often present in BB emissions. IP smoke contained the highest MW HCs of all burns with alkanes and 1-alkenes detected up to C_{18} (Tables A1 and 2). This is consistent with the relative MCEs (Table A1) because smoldering combustion tends to generate higher MW compounds (Lobert and Warnatz, 1993).

Aliphatic HCs were well separated according to DBE; thus the relative contribution of saturated and unsaturated HCs can be readily assessed (Fig. 9). The CG fire emitted the highest fraction of unsaturated compounds, with only one alkane detected; in contrast, IP combustion led predominantly to saturated alkanes (Fig. 9, Table A1). Emissions for the other four fuels fell between CG and IP smoke, with three to eight times higher levels of 1-DBE compounds than saturated compounds (Fig. 9). Of the 1-DBE compounds, the most abundant isomers were generally 1-alkenes; at $\geq C_{13}$, 1-alkenes were often the only unsaturated compounds detected (Tables A1 and 2).

Whereas the aliphatic HC emissions from most fuels were composed primarily of 1- and 2-DBE compounds, 3-DBE compounds constituted the highest fraction of aliphatic HCs in the CG fire emissions (Fig. 9). This class was dominated by 1,3-cyclopentadiene and its methyl derivatives (Table A1). 1,3-Cyclopentadiene may form via loss of CO from phenol (a product of lignin pyrolysis, as discussed in Sect. 3.3.2) and is thought to contribute to the formation of PAHs (e.g., naphthalene) and similar compounds (e.g., indene) during combustion (Fitzpatrick et al., 2008; Mulholland et al., 2000). This is consistent with the high relative contributions from phenolic compounds and PAHs in CG emissions (Fig. 3) and suggests that CG has high lignin content (discussed further in Sect. 3.3.6).

Much recent research has probed the SOA formation potential of aliphatic HCs as a function of carbon number and structure. The SOA yield of alkanes increases dramatically with increasing carbon number – particularly for $> C_{10}$ compounds (Lim and Ziemann, 2009); for example, yields of ~ 50 % (Presto et al., 2010) to ~ 90 % (Lim and Ziemann, 2009); have been reported for heptadecane in the presence of NO_x . Further, the SOA yields of linear alkanes are greater than branched alkanes (Ziemann,

2011). Unsaturated aliphatic HCs are more reactive toward OH and nitrate radical than alkanes, and are susceptible to reaction by ozone. The SOA yield from 1-alkenes is generally higher than alkanes up to C₁₂, at which point the yield of 1-alkenes plateaus (Ziemann, 2011). Terminal alkenes generally exhibit higher SOA yields than internal alkenes, due to a greater propensity for the latter to fragment during oxidation (Ziemann and Atkinson, 2012; Matsunaga et al., 2009). The aliphatic HC isomers most likely to generate significant SOA (i.e., *n*-alkanes and 1-alkenes) were those predominantly observed in the sampled BB emissions: of the non-grass fuels (the grass-derived smoke did not contain significant intermediate volatility aliphatic HCs), the fraction of \geq C₁₀ alkanes that are linear ranged from 68 % (IP) to 87 % (BS) and the fraction of \geq C₁₀ alkenes with a terminal double bond varied from 59 % (IP) to 93 % (BS) (Table A1).

3.3.4 Oxygenated aliphatic compounds

The relative contributions of oxygenated aliphatic compounds to the measured total EF from each burn varied by fuel, from \sim 10 % for IP to \sim 31 % for WG and RS. For the compounds detected here, the dominant oxygenated compounds across all fuels were low MW ketones and aldehydes (Figs. 1–6). These emissions include acyclic compounds, as well as many cyclopentenone derivatives, and cyclopentene-dione isomers (Table A1). Such compounds can arise from the pyrolysis of glucose (Paine et al., 2008a).

RS emissions were dominated by oxygenated compounds (Fig. 5), which can be readily observed by the broad smearing of polar compounds along the secondary axis of the chromatogram. Interestingly, the RS sample had the highest ash content of all fuels tested (7.7 % vs. 1.5–3.8 % by weight; Table A1). Pyrolysis experiments have demonstrated that ash can catalyse cellulose degradation leading to greater yields of several light oxygenated compounds (Patwardhan et al., 2010; Eom et al., 2013, 2012), including hydroxyacetone whose EF is \sim 10-fold higher from RS than any other fuel (Table A1). Thus the disproportionately high ash content in RS may explain the preponderance of the light oxygenated compounds in the BB emissions from this fuel.

23255

Several of the identified ketones and aldehydes are known SOA precursors, such as methyl vinyl ketone (Chan et al., 2013; Liu et al., 2012) and methacrolein (Chan et al., 2010; Surratt et al., 2006). Methacrolein and other unsaturated aldehydes observed in the cartridge samples (e.g., 2-butenal; Table A1) have been shown in laboratory studies to produce SOA through peroxy acyl nitrate (PAN) intermediates, with SOA yields increasing with increasing NO₂/NO ratios (Chan et al., 2010). At the NO₂/NO EF ratios of \sim 3.5–7 reported from ambient BB (Akagi et al., 2013; Simpson et al., 2011) the SOA yield of methacrolein, for example, is reportedly \sim 19–24 % compared to $<$ 3 % under high NO conditions (Chan et al., 2010). Further, \sim 40 % of NO_x has been observed to rapidly form PANs in boreal fire plumes (Alvarado et al., 2010). These observations suggest that unsaturated aldehydes have the potential to form significant SOA via the PAN pathway in BB smoke. Although the available SOA yields of oxygenated aliphatic compounds are generally relatively low ($<$ 10 %), the generated SOA mass may not be trivial in smoke plumes with a high fraction of oxygenated aliphatic compounds (e.g., as from RS).

3.3.5 Terpenoids

Figures 1b and 2b illustrate the significant levels of terpenoids detected in smoke from both coniferous fuels (BS, 27 % and PP, 14 %). The relative contributions of terpenoids from the other fuels were small, and were dominated by isoprene. Isoprene was the only terpene detected in the smoke of all plant fuels sampled (Table A1). Detection of isoprene from burning peat and non-isoprene emitting plants such as RS (Kesselmeier and Staudt, 1999) indicates that isoprene is formed during combustion.

Terpenoids constituted the largest category in BS smoke by EF, but only the fourth largest in PP (Figs. 1 and 2). The BS sample was cut a few days prior to burning and thus should be representative of living BS trees. In contrast, the PP branches were cut approximately one month before the burn and included a mix of brown and green needles. The PP sample therefore represents a mix of forest floor litter and fresh, live branches. Some losses (e.g., through volatilization) of biogenic compounds may

23256

have occurred while storing the PP sample. A more rigorous comparison of the relative magnitudes of terpene emissions should ideally utilize branches of similar freshness. However, both fresh and aged needles (litter) can be important fuel components of fires in coniferous ecosystems (Stockwell et al., 2014; Yokelson et al., 2013); the data reported thus are useful for understanding the smoke from such fires.

In this study, 32 monoterpene (MT) isomers were detected in the smoke from each coniferous fire, of which 13 were positively identified (Table A1). Prior to this work Ciccioli et al. (2001) presented the most comprehensive list of MTs from BB, reporting 14 MTs during a laboratory burn of *Pinus pinea* using GC/MS. In FLAME-4, the 10 most abundant MTs represented ~ 90 % of the total MT emissions for each coniferous fuel, including many of the compounds measured by Ciccioli et al. (2001). Consistency in the MT emissions from a given plant species is suggested by the similarity in the MT-isomer distribution from the BS fire emissions shown in Fig. 10 and a separate BS fire (see Fig. S2 in the Supplement). The relative proportions of the top 10 MT isomers from each fuel are shown in Fig. 10, compared to those previously measured in the corresponding plant essential oils (Krauze-Baranowska et al., 2002; Anderson et al., 1969; von Rudloff, 1975). Camphene (3-carene) is the dominant MT isomer in BS needles (wood), whereas β -pinene (3-carene) is the dominant MT isomer in PP needles (wood) (Fig. 10). Although there is quite reasonable agreement between the MT composition of essential oils and the smoke samples from the coniferous fuels, the relative proportions of MTs in the smoke samples are not exact matches to the essential oils. First, the distribution of MTs differs considerably between the needle- and wood-derived essential oils of these conifers; for example 3-carene is significantly higher in wood than needles (Fig. 10). The relative mass of needles vs. wood burned in these experiments was not measured, but visual observations indicated that needle combustion dominated. This is consistent with the measured distribution of MT isomers in the needle and twig-derived essential oils (e.g., comparing camphene and 3-carene in BS smoke). Further, it is known that MTs can thermally isomerize during pyrolysis (Stolle et al., 2009 and references therein). In particular, myrcene and limonene are known

23257

thermal rearrangement products of β -pinene (Stolle et al., 2009). This may explain the lower relative concentration of β -pinene and higher relative proportions of myrcene and limonene in PP smoke compared to the MT distribution of needle and wood essential oils.

The similarities between the MTs in smoke and those in essential oils demonstrate that MT emissions from BB are plant specific. Because terpenes are essentially distilled out of storage reservoirs during fires (Yokelson et al., 1996), essential oils obtained by steam distillation are likely to be good proxies when predicting MT emissions from BB. For example, the BS essential oil data (von Rudloff, 1975) were also useful for confirming the identification of monoterpenoids detected in BS smoke, including bornyl acetate ($C_{12}H_{20}O_2$) and santene (C_9H_{14}) (Table A1). Although only two coniferous fuels were examined in this work, the major MTs (limonene and α -pinene) observed by Ciccioli et al. (2001) are also in agreement with the major constituents of *Pinus pinea* essential oil (Nasri et al., 2011). Although promising, the reproducibility of such correlations should be confirmed by testing a wider range of plant species and burn conditions.

Given the wide range of atmospheric reactivity and SOA yields among the MT isomers (Lee et al., 2006; Atkinson and Arey, 2003), the variability in MT isomers emitted from different plant species could significantly impact BB SOA chemistry. The compounds included in Fig. 10 have been arranged in order of increasing SOA yields, based largely on Lee et al. (2006) for reaction with OH. As discussed by Akagi et al. (2013), reaction with OH is likely the dominant MT oxidation pathway in smoke plumes. The SOA yield for reaction of camphene with OH has not been characterized; however its SOA yield with ozone is reportedly negligible (Hatfield and Hartz, 2011). Tricyclene does not contain double bonds; its SOA formation potential is assumed here to be the lowest of the MT isomers. Although $1.4\times$ higher total MT EFs were observed for BS (Figs. 1 and 2), BS smoke contained predominantly low SOA-yield MTs, whereas PP-derived smoke contained higher SOA-yield MTs (Fig. 10). For comparison, Fig. 10 also presents the relative MT EFs for “coniferous canopy” fuels listed in the compilation by Yokelson et al. (2013). The average “coniferous canopy” values do not adequately

23258

represent the distribution of either BS or PP, particularly the contributions of the high SOA-yield species, such as limonene. More accurate model predictions of MT-derived SOA likely will be achieved with knowledge of the actual distribution of MT isomers emitted in BB smoke, which will vary among different plant species. At least for MTs, utilizing regional averages or relying solely on PTRMS measurements may not be sufficient for representing SOA formation in air quality and climate applications. Prediction errors may be significant considering the large contribution of these species in the smoke of coniferous fuels (Figs. 1 and 2). In the absence of speciated MT measurements, we propose that SOA models that apply the MT distribution from needle-derived essential oils corresponding to the vegetation mix (if available) will generally yield more reliable results than models assuming a single lumped MT.

Limited information has been reported regarding the speciation of sesquiterpenes (SQTs) in BB smoke. Ciccioli et al. (2001) detected four SQT isomers from burning *Pinus pinea*, but only aromadendrene was identified. Other reports of SQTs in BB smoke are typically derived from PTRMS measurements (e.g., Yokelson et al., 2013), and thus do not provide structural information. SQTs have historically been difficult to measure due to their relatively low volatilities and high reactivities (Pollmann et al., 2005; Bouvier-Brown et al., 2009). However, Pollmann et al. (2005) found no significant adsorption losses of SQTs to a thiosulfate-impregnated filter, as well as high recovery of all isomers from Tenax TA sorbent cartridges. Therefore, SQT-related sampling artifacts were likely minimized in the sampling configuration used in this work, although losses to the Teflon sampling line were not characterized. Highly reactive SQTs may have been partially lost if ozone was not completely removed (Pollmann et al., 2005); however that is unlikely given the negligible ozone concentrations present in fresh BB smoke (Yokelson et al., 2003; Akagi et al., 2013).

Eleven SQT isomers were detected in smoke from the coniferous fuels (Table A1). These GC \times GC measurements therefore reflect the most comprehensive characterization of SQTs in BB smoke to date. No SQTs were found in smoke from the other fuels, however the IP fire emitted SQT-like compounds with the formula $C_{15}H_{26}$ (Table A1).

23259

Sesquiterpenes constituted a small fraction of the terpenes observed in both BS and PP (Figs. 1 and 2), consistent with the relatively low levels present in these essential oils (Krauze-Baranowska et al., 2002; von Rudloff, 1975). The majority of the observed SQTs are tentatively identified as isomers of cadinene, amorphene, and/or muurolene, which have the same bi-cyclic cadalane skeleton and differ only in the position of the two double bonds and stereochemistry; these are labelled as cadinene isomers in Table A1. Cadinene isomers have been previously detected in the essential oils of BS (von Rudloff, 1975) and PP (Krauze-Baranowska et al., 2002). Other tentatively identified compounds with a cadalane backbone were also observed, including copaene ($C_{15}H_{24}$), calamenene ($C_{15}H_{22}$), and calacorene ($C_{15}H_{20}$) (Table A1). Cadinenes have received comparatively little study in terms of atmospheric reactivity; however other SQT isomers are known to have high SOA yields (Lee et al., 2006).

3.3.6 Furans

Although furans are oxygenated aromatic species, a separate class was created since they constituted a significant fraction (5–37 %) of the smoke from each fuel tested (Figs. 1–6). Furans arise primarily from the breakdown and dehydration of cellulose (Paine et al., 2008b). Compounds in this group generally contained 4–6 carbons with alkyl and/or oxygenated substituents, most commonly as aldehyde or alcohol moieties (Table A1). Furan emissions were generally dominated by furan and furfural, with significant contributions from 2-methyl furan and 2-furanmethanol (Figs. 1–6, Table A1).

Wiregrass smoke contained the highest relative furan contribution (37 %, Fig. 4). Furfural was the dominant species emitted from this fuel within the range of analyzed compounds (Table A1). In contrast, CG combustion emitted largely benzene and naphthalene derivatives (Fig. 3). The variation in emissions could indicate substantial differences in the structure of these grasses: the high levels of furans detected in WG smoke suggests high levels of cellulose in the plant material whereas the preponderance of aromatic compounds, including phenols, in CG smoke suggest high lignin content as discussed above (Sect. 3.3.1). This hypothesis is consistent with the structures of these

23260

plants. Giant cutgrass is characterized by tall, wide, and stiff leaves that likely require higher lignin content for support. In comparison, wiregrass is short, wiry, and flimsy. Although the biomass composition of these grasses have not been measured, Ortega et al. (2013) reported that the fraction of particle-phase levoglucosan (as f_{60} in their aerosol mass spectrometry measurements) – a known product in cellulose degradation – was higher in WG smoke than other fuels tested except sawgrass, consistent with the hypothesis of high cellulose content in WG. The MCEs were quite different for these two burns (0.925 for CG vs. 0.97 for WG) and thus combustion conditions may also have influenced the emitted compounds.

Furans are highly reactive, with atmospheric lifetimes on the order of several hours with respect to OH oxidation (Bierbach et al., 1992). Although the kinetics of furfural oxidation have been characterized (Colmenar et al., 2012; Bierbach et al., 1995), product studies have not yet been conducted, thereby limiting assessment of its SOA-formation potential. Gas-phase photochemistry of alkyl furans has been more extensively studied (Alvarado et al., 1996; Aschmann et al., 2011; Bierbach et al., 1992; Gómez Alvarez et al., 2009) and generally proceeds via OH-radical addition to the aromatic ring with subsequent ring opening (Bierbach et al., 1995). The major identified products are unsaturated-1,4 dicarbonyls, with yields that decrease with increasing number of alkyl substituents (Aschmann et al., 2014). Strollo and Ziemann (2013) found that these first-generation reaction products of 3-methyl furan can undergo acid-catalyzed condensed-phase oligomerization reactions, with SOA yields up to 15 %. Given that aldehydes are more likely to oligomerize than ketones (Strollo and Ziemann, 2013), furan and 3-methyl furan will likely produce the highest SOA yields by this mechanism since their predominant first generation products are unsaturated dialdehydes (Aschmann et al., 2014). These unsaturated aldehydes may also react through a PAN channel, as discussed in Sect. 3.3.4. Given the high levels of furans detected in these smoke samples, it is important to elucidate the potential SOA formation pathways of these compounds and their role in SOA production in BB plumes.

23261

3.3.7 Nitrogen- and sulfur-containing compounds

Emissions of N- and S-containing compounds are generally proportional to the nitrogen and sulfur content of the fuel biomass (Ward, 1990). Consistent with the relative nitrogen content in the fuels (Table A1), giant cutgrass smoke had the highest relative contribution from N-containing species: 11 % vs. ~ 2–6 % from the other fuels. The predominant emitted N-species from CG combustion were nitriles that arise from the pyrolysis of amino acids (Lobert and Warnatz, 1993). Interestingly, the predominant N-containing species from most other fuels was pyrrole rather than nitriles. However, acetonitrile was likely underestimated by our measurements due to high breakthrough. Extensive N-heterocyclic compounds have also been observed in PM samples from burns of RS (Ma and Hays, 2008) and PP (Laskin et al., 2009), consistent with the observations herein. The SOA-formation potentials of pyrroles and nitrile have not been elucidated. However, due to the small molecular sizes and relatively low concentrations of the observed compounds, they are not likely to contribute significantly to BB SOA.

Sulfur is an important nutrient for plant physiology. As discussed by Ward (1990), sulfur in ecosystems can only be replenished through deposition; thus losses of sulfur due to fire activity can influence land sustainability and sulfur transport. Thiophene – the sulfur analog to furan – and its derivatives were detected in five of the fuels tested. To our knowledge, only Ciccioli et al. (2001) have identified thiophene in BB emissions, however they do not report an EF. Dimethyl sulfide (DMS) and dimethyl disulfide are the predominant organosulfur compounds that have been reported in BB smoke to date (Akagi et al., 2011; Simpson et al., 2011; Friedli et al., 2001; Meinardi et al., 2003). In this work, the thiophene EF has been quantified, along with its methyl and benzo(a)thiophene derivatives. The reported thiophene EFs are comparable to the EFs commonly reported for DMS (Akagi et al., 2011; Simpson et al., 2011), therefore thiophenes may be important organosulfur species in BB emissions. (Dimethyl disulfide was detected at trace levels in the RS burn, but was not quantified due to lack of a suitable standard compound.) Rate constants for reactions of thiophene with atmospheric

23262

oxidants have been measured (Atkinson et al., 1983; Cabañas et al., 2005), and are generally slower than the corresponding furan reactions due to greater aromaticity of the thiophene ring compared to furan (Bierbach et al., 1992); SOA yields are unknown.

4 Conclusions

5 This work represents the first application of GC × GC/TOFMS for the broad characterization of NMOCs from biomass burning. Utilizing the approach described herein, 722 total compounds in the C₂-C₁₈ range were speciated, including the cartridge and filter-desorption samples, demonstrating the extensive capability of GC × GC/TOFMS to facilitate identification and quantification of BB emissions. Although the ability to reliably
10 quantify analytes present at very high concentrations (e.g., benzene) was hindered due to limited dynamic range, newer model ATD instruments permit trapping of the unused portion of each sample, thereby enabling multiple analyses of each cartridge sample. In particular, application of different GC × GC inlet split ratios would extend the range of quantitation and different column sets could be used to target more or less polar species. Further, alternative sorbent beds could be utilized for ATD cartridge sampling
15 to target different volatility ranges, as desired (Pankow et al., 2012, 1998). This method is highly complementary to the other instrumentation commonly utilized for NMOC determinations. PTR-MS can measure some polar species not amenable to analysis by GC and in real time, but is limited in the area of compound identification due to the sole
20 reliance on mass-to-charge ratio. In contrast, canister sampling with 1D-GC analysis is ideal for compounds that breakthrough ATD cartridges, but 1D-GC cannot separate a large number of compounds. All of these approaches, in addition to OP-FTIR, were utilized during FLAME-4 (Stockwell et al., 2014) and the measurements will be synthesized in future work.

25 The 722 compounds positively/tentatively identified across six laboratory burns afforded unique insights into gas-phase BB emissions. In particular, the identified compounds could be related to the plant composition in a number of ways. The high levels of

23263

aromatic hydrocarbons and cyclopentadienes in giant-cutgrass smoke imply high lignin content in this grass species compared to wiregrass, which appears to be more cellulosic in structure based on the high furan emissions. Additionally, the thorough characterization of terpenoids emitted by burning conifer branches allowed direct correlations
5 to be made between BB emissions and the corresponding essential oils, underscoring that emissions of terpenoid isomers will be specific to individual plant species/fuel types. These measurements have also provided the first comprehensive characterization of intermediate volatility alkanes/alkenes in BB, with compounds up to C₁₅ present in most smoke samples and as high as C₁₈ in the case of the Indonesian peat fire.
10 Separation of hydrocarbons by double bond equivalents further illustrated a high degree of unsaturation among aliphatic compounds, which will be highly reactive toward atmospheric oxidants. Overall, the distribution of emissions among different compound classes was found to vary considerably from fuel to fuel, indicating that the dominant reaction pathways in aging plumes will be highly dependent on the burned fuel types.

15 These comprehensive measurements have elucidated a large number of potential SOA precursors in BB emissions, including abundant isomers of aliphatic and aromatic hydrocarbons, phenol derivatives, monoterpenes, and sesquiterpenes. To estimate the relative importance of different precursor classes, the potential SOA mass from each category has been calculated using published SOA yields and assuming that all precursors react completely (Table 3). For all fuels, aromatic hydrocarbons are predicted
20 to produce the largest fraction of SOA, ranging from 33 % (WG) to 84 % (CG). The terpenes are also expected to contribute significantly to SOA in emissions from coniferous fuels and account for 24 and 36 % of the calculated SOA mass for PP and BS, respectively. SOA produced from aliphatic hydrocarbons was assumed to result from ≥ C₉
25 compounds only; the calculated SOA was significant for Indonesian peat BB emissions only due to the higher molecular weight species observed in this sample (Sect. 3.3.3). In addition to these common SOA precursors, recent research has demonstrated the potential for furans to contribute to SOA formation (Strollo and Ziemann, 2013), indicating that furans may be a previously unconsidered class of SOA precursors in BB

23264

smoke. We have assumed 10 % SOA yields for all furan derivatives, based on the measured yield of 3-methyl furan (Strollo and Ziemann, 2013). At this SOA yield, furans may produce non-trivial SOA mass, including about one-third of the SOA calculated from WG emissions (Table 3). However, because the SOA-formation potential of furfural (the dominant furan derivative in BB emissions) has not been studied, it is unclear if the predicted furan-derived SOA is significantly over or underestimated. Overall, the identified SOA precursors produce estimated OA enhancement ratios on the order of 1.02–1.2, which is a lower limit based on detected compounds and in the range of that reported for laboratory experiments (Hennigan et al., 2011; Ortega et al., 2013) and ambient BB plumes (Akagi et al., 2012; Yokelson et al., 2009). Because BB dominates global fine POA emissions, even modest enhancements can represent significant production of OA mass.

Despite the range of possible SOA precursors, most atmospheric models treat SOA formation through condensation of surrogates representing the gas-phase oxidation products of a very small number of NMOCs, which typically include benzene, toluene, xylenes, and select biogenic compounds (Odum et al., 1996; Kanakidou et al., 2005; Henze et al., 2008). Such simplified representations cannot adequately capture the diversity in emissions and plume chemistry that is to be expected based on these GC \times GC/TOFMS measurements and other recent efforts (Yokelson et al., 2013). Indeed, recent modeling studies were unable to recreate measured OA levels in BB plumes or BB-influenced regions (Alvarado et al., 2009; Heald et al., 2011), demonstrating that additional precursors and/or formation mechanisms need to be considered. These comprehensive GC \times GC/TOFMS emissions measurements provide a significant step in that direction by identifying and quantifying extensive potential SOA precursors. The reported EFs can further supplement the existing BB emission inventories (van der Werf et al., 2010; Wiedinmyer et al., 2011; Akagi et al., 2011) that provide the input for atmospheric BB models. Although computational limits will preclude describing the chemistry of 700+ primary species for the foreseeable future, a subset of the major, ubiquitous species determined herein can serve to focus future modelling efforts.

23265

**The Supplement related to this article is available online at
doi:10.5194/acpd-14-23237-2014-supplement.**

Acknowledgements. Melissa Roskamp (Portland State University) is thanked for assistance in sampling preparations and testing the ozone scrubbing efficiency of the sodium-thiosulfate impregnated filters. Additional assistance from Lorne Isabelle (Portland State University) is also appreciated. Sonia Kreidenweis and Paul DeMott (Colorado State University) are thanked for helping to coordinate the FLAME-4 campaign. This work was supported by a National Science Foundation Atmospheric and Geospace Sciences Postdoctoral Research Fellowship (Grant # 1231128). Additionally, FLAME-4, C. S., and R. Y. were supported by NSF grant ATM-0936321.

References

- Aiken, A. C., Decarlo, P. F., Kroll, J. H., Worsnop, D. R., Huffman, J. A., Docherty, K. S., Ulbrich, I. M., Mohr, C., Kimmel, J. R., Sueper, D., Sun, Y., Zhang, Q., Trimborn, A., Northway, M., Ziemann, P. J., Canagaratna, M. R., Onasch, T. B., Alfarra, M. R., Prevot, A. S. H., Dommen, J., Duplissy, J., Metzger, A., Baltensperger, U., and Jimenez, J. L.: O/C and OM/OC ratios of primary, secondary, and ambient organic aerosols with high-resolution time-of-flight aerosol mass spectrometry, *Environ. Sci. Technol.*, 42, 4478–4485, doi:10.1021/Es703009q, 2008.
- Akagi, S. K., Yokelson, R. J., Wiedinmyer, C., Alvarado, M. J., Reid, J. S., Karl, T., Crounse, J. D., and Wennberg, P. O.: Emission factors for open and domestic biomass burning for use in atmospheric models, *Atmos. Chem. Phys.*, 11, 4039–4072, doi:10.5194/acp-11-4039-2011, 2011.
- Akagi, S. K., Craven, J. S., Taylor, J. W., McMeeking, G. R., Yokelson, R. J., Burling, I. R., Urbanski, S. P., Wold, C. E., Seinfeld, J. H., Coe, H., Alvarado, M. J., and Weise, D. R.: Evolution of trace gases and particles emitted by a chaparral fire in California, *Atmos. Chem. Phys.*, 12, 1397–1421, doi:10.5194/acp-12-1397-2012, 2012.
- Akagi, S. K., Yokelson, R. J., Burling, I. R., Meinardi, S., Simpson, I., Blake, D. R., McMeeking, G. R., Sullivan, A., Lee, T., Kreidenweis, S., Urbanski, S., Reardon, J., Griffith, D. W. T., Johnson, T. J., and Weise, D. R.: Measurements of reactive trace gases and variable O₃ formation rates in some South Carolina biomass burning plumes, *Atmos. Chem. Phys.*, 13, 1141–1165, doi:10.5194/acp-13-1141-2013, 2013.

23266

- Alvarado, A., Atkinson, R., and Arey, J.: Kinetics of the gas-phase reactions of NO₃ radicals and O₃ with 3-methyl furan and the OH radical yield from the O₃ reaction, *Int. J. Chem. Kinet.*, 28, 905–909, 1996.
- Alvarado, M. J., Wang, C., and Prinn, R. G.: Formation of ozone and growth of aerosols in young smoke plumes from biomass burning: 2. Three-dimensional Eulerian studies, *J. Geophys. Res.-Atmos.*, 114, D09307, doi:10.1029/2008jd011186, 2009.
- Alvarado, M. J., Logan, J. A., Mao, J., Apel, E., Riemer, D., Blake, D., Cohen, R. C., Min, K.-E., Perring, A. E., Browne, E. C., Wooldridge, P. J., Diskin, G. S., Sachse, G. W., Fuelberg, H., Sessions, W. R., Harrigan, D. L., Huey, G., Liao, J., Case-Hanks, A., Jimenez, J. L., Cubison, M. J., Vay, S. A., Weinheimer, A. J., Knapp, D. J., Montzka, D. D., Flocke, F. M., Pollock, I. B., Wennberg, P. O., Kurten, A., Crounse, J., Clair, J. M. St., Wisthaler, A., Mikoviny, T., Yantosca, R. M., Carouge, C. C., and Le Sager, P.: Nitrogen oxides and PAN in plumes from boreal fires during ARCTAS-B and their impact on ozone: an integrated analysis of aircraft and satellite observations, *Atmos. Chem. Phys.*, 10, 9739–9760, doi:10.5194/acp-10-9739-2010, 2010.
- Anderson, A. B., Riffer, R., and Wong, A.: Monoterpenes fatty and resin acids of *Pinus Ponderosa* and *Pinus Jeffreya*, *Phytochemistry*, 8, 873–875, doi:10.1016/S0031-9422(00)85876-8, 1969.
- Andreae, M. O. and Merlet, P.: Emission of trace gases and aerosols from biomass burning, *Global Biogeochem. Cy.*, 15, 955–966, 2001.
- Andreae, M. O., Rosenfeld, D., Artaxo, P., Costa, A. A., Frank, G. P., Longo, K. M., and Silva-Dias, M. A. F.: Smoking rain clouds over the Amazon, *Science*, 303, 1337–1342, doi:10.1126/Science.1092779, 2004.
- Aschmann, S. M., Nishino, N., Arey, J., and Atkinson, R.: Kinetics of the reactions of OH radicals with 2- and 3-methylfuran, 2,3- and 2,5-dimethylfuran, and E- and Z-3-hexene-2,5-dione, and products of OH + 2,5-dimethylfuran, *Environ. Sci. Technol.*, 45, 1859–1865, doi:10.1021/es103207k, 2011.
- Aschmann, S. M., Nishino, N., Arey, J., and Atkinson, R.: Products of the OH radical-initiated reactions of Furan, 2-and 3-Methylfuran, and 2,3-and 2,5-Dimethylfuran in the presence of NO, *J. Phys. Chem. A*, 118, 457–466, 2014.
- Atkinson, R. and Arey, J.: Gas-phase tropospheric chemistry of biogenic volatile organic compounds: a review, *Atmos. Environ.*, 37, S197–S219, 2003.

23267

- Atkinson, R., Aschmann, S. M., and Carter, W. P. L.: Kinetics of the reaction of O₃ and OH radicals with Furan and Thiophene at 298 ± 2 K, *Int. J. Chem. Kinet.*, 15, 51–61, 1983.
- Beens, J., Tijssen, R., and Blomberg, J.: Prediction of comprehensive two-dimensional gas chromatographic separations – a theoretical and practical exercise, *J. Chromatogr. A*, 822, 233–251, 1998.
- Bierbach, A., Barnes, I., and Becker, K. H.: Rate coefficients for the gas-phase reactions of hydroxyl radicals with furan, 2-methylfuran, 2-ethylfuran, and 2,5-dimethylfuran, *Atmos. Environ.*, 26, 813–817, 1992.
- Bierbach, A., Barnes, I., and Becker, K. H.: Product and kinetic study of the OH-initiated gas-phase oxidation of furan, 2-methylfuran, and furan aldehydes at 300 K, *Atmos. Environ.*, 29, 2651–2660, 1995.
- Bouvier-Brown, N. C., Goldstein, A. H., Gilman, J. B., Kuster, W. C., and de Gouw, J. A.: In-situ ambient quantification of monoterpenes, sesquiterpenes, and related oxygenated compounds during BEARPEX 2007: implications for gas- and particle-phase chemistry, *Atmos. Chem. Phys.*, 9, 5505–5518, doi:10.5194/acp-9-5505-2009, 2009.
- Brockway, D. G. and Lewis, C. E.: Long-term effects of dormant-season prescribed fire on plant community diversity, structure and productivity in a longleaf pine wiregrass ecosystem, *Forest Ecol. Manag.*, 96, 167–183, 1997.
- Cabañas, B., Baeza, M. T., Martín, P., Salgado, S., Villanueva, F., Monedero, E., and Wirtz, K.: Products and mechanism of the NO₃ reaction with thiophene, *J. Atmos. Chem.*, 51, 317–335, doi:10.1007/s10874-005-3580-5, 2005.
- Chan, A. W. H., Kautzman, K. E., Chhabra, P. S., Surratt, J. D., Chan, M. N., Crounse, J. D., Kürten, A., Wennberg, P. O., Flagan, R. C., and Seinfeld, J. H.: Secondary organic aerosol formation from photooxidation of naphthalene and alkylnaphthalenes: implications for oxidation of intermediate volatility organic compounds (IVOCs), *Atmos. Chem. Phys.*, 9, 3049–3060, doi:10.5194/acp-9-3049-2009, 2009.
- Chan, A. W. H., Chan, M. N., Surratt, J. D., Chhabra, P. S., Loza, C. L., Crounse, J. D., Yee, L. D., Flagan, R. C., Wennberg, P. O., and Seinfeld, J. H.: Role of aldehyde chemistry and NO_x concentrations in secondary organic aerosol formation, *Atmos. Chem. Phys.*, 10, 7169–7188, doi:10.5194/acp-10-7169-2010, 2010.

23268

- Chan, K. M., Huang, D. D., Li, Y. J., Chan, M. N., Seinfeld, J. H., and Chan, C. K.: Oligomeric products and formation mechanisms from acid-catalyzed reactions of methyl vinyl ketone on acidic sulfate particles, *J. Atmos. Chem.*, 70, 1–18, doi:10.1007/S10874-013-9248-7, 2013.
- Chang, D. and Song, Y.: Estimates of biomass burning emissions in tropical Asia based on satellite-derived data, *Atmos. Chem. Phys.*, 10, 2335–2351, doi:10.5194/acp-10-2335-2010, 2010.
- Christian, T. J., Kleiss, B., Yokelson, R. J., Holzinger, R., Crutzen, P. J., Hao, W. M., Saharjo, B. H., and Ward, D. E.: Comprehensive laboratory measurements of biomass-burning emissions: 1. Emissions from Indonesian, African, and other fuels, *J. Geophys. Res.-Atmos.*, 108, 4719, doi:10.1029/2003jd003704, 2003.
- Christian, T. J., Kleiss, B., Yokelson, R. J., Holzinger, R., Crutzen, P. J., Hao, W. M., Shirai, T., and Blake, D. R.: Comprehensive laboratory measurements of biomass-burning emissions: 2. First intercomparison of open-path FTIR, PTR-MS, and GC-MS/FID/ECD, *J. Geophys. Res.-Atmos.*, 109, D02311, doi:10.1029/2003jd003874, 2004.
- Ciccioli, P., Brancaleoni, E., Frattoni, M., Cecinato, A., and Pinciarelli, L.: Determination of volatile organic compounds (VOC) emitted from biomass burning of Mediterranean vegetation species by GC-MS, *Anal. Lett.*, 34, 937–955, 2001.
- Colmenar, I., Cabañas, B., Martínez, E., Salgado, M. S., and Martín, P.: Atmospheric fate of a series of furan-aldehydes by their NO₃ reactions, *Atmos. Environ.*, 54, 177–184, doi:10.1016/j.atmosenv.2012.02.087, 2012.
- Crutzen, P. J. and Andreae, M. O.: Biomass burning in the tropics – impact on atmospheric chemistry and biogeochemical cycles, *Science*, 250, 1669–1678, 1990.
- Cumming, S. G.: Forest type and wildfire in the alberta boreal mixedwood: what do fires burn?, *Ecol. Appl.*, 11, 97–110, 2001.
- Desalmand, F. and Serpolay, R.: Some specific features of the aerosol-particle concentrations during the dry season and during a bushfire event in West-Africa, *Atmos. Environ.*, 19, 1535–1543, 1985.
- Eom, I. Y., Kim, J. Y., Kim, T. S., Lee, S. M., Choi, D., Choi, I. G., and Choi, J. W.: Effect of essential inorganic metals on primary thermal degradation of lignocellulosic biomass, *Bioresource Technol.*, 104, 687–694, doi:10.1016/j.biortech.2011.10.035, 2012.
- Eom, I. Y., Kim, J. Y., Lee, S. M., Cho, T. S., Yeo, H., and Choi, J. W.: Comparison of pyrolytic products produced from inorganic-rich and demineralized rice straw (*Oryza sativa* L.) by

23269

- fluidized bed pyrolyzer for future biorefinery approach, *Bioresource Technol.*, 128, 664–672, doi:10.1016/J.Biortech.2012.09.082, 2013.
- Finlayson-Pitts, B. J. and Pitts, J. N.: *Chemistry of the Upper and Lower Atmosphere: Theory, Experiments, and Applications*, Academic Press, San Diego, 2000.
- Fitzpatrick, E. M., Jones, J. A., Pourkashanian, M., Ross, A. B., Williams, A., and Bartle, K. D.: Mechanistic aspects of soot formation from the combustion of pine wood, *Energy Fuels*, 22, 3771–3778, 2008.
- Friedli, H. R., Atlas, E., Stroud, V. R., Giovanni, L., Campos, T., and Radke, L. F.: Volatile organic trace gases emitted from North American wildfires, *Global Biogeochem. Cy.*, 15, 435–452, 2001.
- Gómez Alvarez, E., Borrás, E., Viidanoja, J., and Hjorth, J.: Unsaturated dicarbonyl products from the OH-initiated photo-oxidation of furan, 2-methylfuran and 3-methylfuran, *Atmos. Environ.*, 43, 1603–1612, doi:10.1016/j.atmosenv.2008.12.019, 2009.
- Grieshop, A. P., Logue, J. M., Donahue, N. M., and Robinson, A. L.: Laboratory investigation of photochemical oxidation of organic aerosol from wood fires 1: measurement and simulation of organic aerosol evolution, *Atmos. Chem. Phys.*, 9, 1263–1277, doi:10.5194/acp-9-1263-2009, 2009.
- Haines, T. K. and Busby, R. L.: Prescribed burning in the South: trends, purpose, and barriers, *Journal of Applied Forestry*, 25, 149–153, 2001.
- Hallquist, M., Wenger, J. C., Baltensperger, U., Rudich, Y., Simpson, D., Claeys, M., Dommen, J., Donahue, N. M., George, C., Goldstein, A. H., Hamilton, J. F., Herrmann, H., Hoffmann, T., Iinuma, Y., Jang, M., Jenkin, M. E., Jimenez, J. L., Kiendler-Scharr, A., Maenhaut, W., McFiggans, G., Mentel, Th. F., Monod, A., Prévôt, A. S. H., Seinfeld, J. H., Surratt, J. D., Szmigielski, R., and Wildt, J.: The formation, properties and impact of secondary organic aerosol: current and emerging issues, *Atmos. Chem. Phys.*, 9, 5155–5236, doi:10.5194/acp-9-5155-2009, 2009.
- Hatfield, M. L. and Hartz, K. E. H.: Secondary organic aerosol from biogenic volatile organic compound mixtures, *Atmos. Environ.*, 45, 2211–2219, 2011.
- Heald, C. L., Coe, H., Jimenez, J. L., Weber, R. J., Bahreini, R., Middlebrook, A. M., Russell, L. M., Jolleys, M., Fu, T.-M., Allan, J. D., Bower, K. N., Capes, G., Crosier, J., Morgan, W. T., Robinson, N. H., Williams, P. I., Cubison, M. J., DeCarlo, P. F., and Dunlea, E. J.: Exploring the vertical profile of atmospheric organic aerosol: comparing 17 aircraft field cam-

23270

- paings with a global model, *Atmos. Chem. Phys.*, 11, 12673–12696, doi:10.5194/acp-11-12673-2011, 2011.
- Heil, A.: Indonesian forest and peat fires: emissions, air quality, and human health, Ph.D. thesis, Max Planck Institute for Meteorology, Hamburg, 142 pp., 2007.
- 5 Helmig, D.: Ozone removal techniques in the sampling of atmospheric volatile organic trace gases, *Atmos. Environ.*, 31, 3635–3651, 1997.
- Hennigan, C. J., Miracolo, M. A., Engelhart, G. J., May, A. A., Presto, A. A., Lee, T., Sullivan, A. P., McMeeking, G. R., Coe, H., Wold, C. E., Hao, W.-M., Gilman, J. B., Kuster, W. C., de Gouw, J., Schichtel, B. A., Collett Jr., J. L., Kreidenweis, S. M., and Robinson, A. L.: Chemical and physical transformations of organic aerosol from the photo-oxidation of open biomass burning emissions in an environmental chamber, *Atmos. Chem. Phys.*, 11, 7669–7686, doi:10.5194/acp-11-7669-2011, 2011.
- 10 Henze, D. K., Seinfeld, J. H., Ng, N. L., Kroll, J. H., Fu, T.-M., Jacob, D. J., and Heald, C. L.: Global modeling of secondary organic aerosol formation from aromatic hydrocarbons: high- vs. low-yield pathways, *Atmos. Chem. Phys.*, 8, 2405–2420, doi:10.5194/acp-8-2405-2008, 2008.
- Hobbs, P. V., Reid, J. S., Kotchenruther, R. A., Ferek, R. J., and Weiss, R.: Direct radiative forcing by smoke from biomass burning, *Science*, 275, 1776–1778, 1997.
- Jiang, G. Z., Nowakowski, D. J., and Bridgwater, A. V.: Effect of the temperature on the composition of lignin pyrolysis products, *Energy Fuels*, 24, 4470–4475, 2010.
- 20 Jolleys, M. D., Coe, H., McFiggans, G., Capes, G., Allan, J. D., Crosier, J., Williams, P. I., Allen, G., Bower, K. N., Jimenez, J. L., Russell, L. M., Grutter, M., and Baumgardner, D.: Characterizing the aging of biomass burning organic aerosol by use of mixing ratios: a meta-analysis of four regions, *Environ. Sci. Technol.*, 46, 13093–13102, 2012.
- 25 Kanakidou, M., Seinfeld, J. H., Pandis, S. N., Barnes, I., Dentener, F. J., Facchini, M. C., Van Dingenen, R., Ervens, B., Nenes, A., Nielsen, C. J., Swietlicki, E., Putaud, J. P., Balkanski, Y., Fuzzi, S., Horth, J., Moortgat, G. K., Winterhalter, R., Myhre, C. E. L., Tsigaridis, K., Vignati, E., Stephanou, E. G., and Wilson, J.: Organic aerosol and global climate modelling: a review, *Atmos. Chem. Phys.*, 5, 1053–1123, doi:10.5194/acp-5-1053-2005, 2005.
- 30 Kesselmeier, J. and Staudt, M.: Biogenic volatile organic compounds (VOC): an overview on emission, physiology and ecology, *J. Atmos. Chem.*, 33, 23–88, 1999.

23271

- Krauze-Baranowska, M., Mardarowicz, M., Wiwart, M., Poblocka, L., and Dynowska, M.: Antifungal activity of the essential oils from some species of the genus *Pinus*, *Z. Naturforsch. C*, 57, 478–482, 2002.
- Kroll, J. H. and Seinfeld, J. H.: Chemistry of secondary organic aerosol: formation and evolution of low-volatility organics in the atmosphere, *Atmos. Environ.*, 42, 3593–3624, doi:10.1016/j.atmosenv.2008.01.003, 2008.
- 5 Laskin, A., Smith, J. S., and Laskin, J.: Molecular characterization of nitrogen-containing organic compounds in biomass burning aerosols using high-resolution mass spectrometry, *Environ. Sci. Technol.*, 43, 3764–3771, 2009.
- 10 Lee, A., Goldstein, A. H., Kroll, J. H., Ng, N. L., Varutbangkul, V., Flagan, R. C., and Seinfeld, J. H.: Gas-phase products and secondary aerosol yields from the photooxidation of 16 different terpenes, *J. Geophys. Res.*, 111, D17305, doi:10.1029/2006jd007050, 2006.
- Lim, Y. B. and Ziemann, P. J.: Effects of molecular structure on aerosol yields from OH radical-initiated reactions of linear, branched, and cyclic alkanes in the presence of NO_x, *Environ. Sci. Technol.*, 43, 2328–2334, doi:10.1021/Es803389s, 2009.
- 15 Liu, Y., Siekmann, F., Renard, P., El Zein, A., Salque, G., El Haddad, I., Temime-Roussel, B., Voisin, D., Thissen, R., and Monod, A.: Oligomer and SOA formation through aqueous phase photooxidation of methacrolein and methyl vinyl ketone, *Atmos. Environ.*, 49, 123–129, doi:10.1016/J.Atmosenv.2011.12.012, 2012.
- 20 Lobert, J. M. and Warnatz, J.: Emissions from the combustion process in vegetation, in: *Fire in the Environment: the Ecological, Atmospheric, and Climatic Importance of Vegetation Fires*, edited by: Crutzen, P. J. and Goldammer, J. G., John Wiley & Sons Ltd., New York, 15–37, 1993.
- Lohmann, U. and Feichter, J.: Global indirect aerosol effects: a review, *Atmos. Chem. Phys.*, 5, 715–737, doi:10.5194/acp-5-715-2005, 2005.
- 25 Ma, Y., Hays, M. D., Geron, C. D., Walker, J. T., and Gatari Gichuru, M. J.: Technical Note: Fast two-dimensional GC-MS with thermal extraction for anhydro-sugars in fine aerosols, *Atmos. Chem. Phys.*, 10, 4331–4341, doi:10.5194/acp-10-4331-2010, 2010.
- Ma, Y. L. and Hays, M. D.: Thermal extraction-two-dimensional gas chromatography-mass spectrometry with heart-cutting for nitrogen heterocyclics in biomass burning aerosols, *J. Chromatogr. A*, 1200, 228–234, doi:10.1016/j.chroma.2008.05.078, 2008.
- 30

23272

- Matsunaga, A., Docherty, K. S., Lim, Y. B., and Ziemann, P. J.: Composition and yields of secondary organic aerosol formed from OH radical-initiated reactions of linear alkenes in the presence of NO_x: modeling and measurements, *Atmos. Environ.*, 43, 1349–1357, 2009.
- McMeeking, G. R., Kreidenweis, S. M., Baker, S., Carrico, C. M., Chow, J. C., Collett, J. L., Hao, W. M., Holden, A. S., Kirchstetter, T. W., Malm, W. C., Moosmuller, H., Sullivan, A. P., and Wold, C. E.: Emissions of trace gases and aerosols during the open combustion of biomass in the laboratory, *J. Geophys. Res.-Atmos.*, 114, D19210, doi:10.1029/2009jd011836, 2009.
- Meinardi, S., Simpson, I. J., Blake, N. J., Blake, D. R., and Rowland, F. S.: Dimethyl disulfide (DMS) and dimethyl sulfide (DMS) emissions from biomass burning in Australia, *Geophys. Res. Lett.*, 30, 1454, 2003.
- Mondello, L., Tranchida, P. Q., Dugo, P., and Dugo, G.: Comprehensive two-dimensional gas chromatography-mass spectrometry: a review, *Mass Spectrom. Rev.*, 27, 101–124, doi:10.1002/Mas.20158, 2008.
- Mulholland, J. A., Lu, M., and Kim, D. H.: Pyrolytic growth of polycyclic aromatic hydrocarbons by cyclopentadienyl moieties, *P. Combust. Inst.*, 28, 2593–2599, 2000.
- Nakao, S., Clark, C., Tang, P., Sato, K., and Cocker III, D.: Secondary organic aerosol formation from phenolic compounds in the absence of NO_x, *Atmos. Chem. Phys.*, 11, 10649–10660, doi:10.5194/acp-11-10649-2011, 2011.
- Nara, H., Nakagawa, F., and Yoshida, N.: Development of two-dimensional gas chromatography/isotope ratio mass spectrometry for the stable carbon isotopic analysis Of C(2)–C(5) non-methane hydrocarbons emitted from biomass burning, *Rapid Commun. Mass. Sp.*, 20, 241–247, doi:10.1002/Rcm.2302, 2006.
- Nasri, N., Tlili, N., Triki, S., Elfalleh, W., Cheraif, I., and Khaldi, A.: Volatile constituents of *Pinus pinea* L. needles, *J. Essent. Oil Res.*, 23, 15–19, 2011.
- Ng, N. L., Kroll, J. H., Chan, A. W. H., Chhabra, P. S., Flagan, R. C., and Seinfeld, J. H.: Secondary organic aerosol formation from *m*-xylene, toluene, and benzene, *Atmos. Chem. Phys.*, 7, 3909–3922, doi:10.5194/acp-7-3909-2007, 2007.
- Oanh, N. T. K., Ly, B. T., Tipayarom, D., Manandhar, B. R., Prapat, P., Simpson, C. D., and Liu, L. J. S.: Characterization of particulate matter emission from open burning of rice straw, *Atmos. Environ.*, 45, 493–502, doi:10.1016/J.Atmosenv.2010.09.023, 2011.
- Odum, J. R., Hoffmann, T., Bowman, F., Collins, D., Flagan, R. C., and Seinfeld, J. H.: Gas/particle partitioning and secondary organic aerosol yields, *Environ. Sci. Technol.*, 30, 2580–2585, doi:10.1021/Es950943+, 1996.

23273

- Ortega, A. M., Day, D. A., Cubison, M. J., Brune, W. H., Bon, D., de Gouw, J. A., and Jimenez, J. L.: Secondary organic aerosol formation and primary organic aerosol oxidation from biomass-burning smoke in a flow reactor during FLAME-3, *Atmos. Chem. Phys.*, 13, 11551–11571, doi:10.5194/acp-13-11551-2013, 2013.
- Page, S. E., Siegert, F., Rieley, J. O., Boehm, H. D. V., Jaya, A., and Limin, S.: The amount of carbon released from peat and forest fires in Indonesia during 1997, *Nature*, 420, 61–65, 2002.
- Paine, J. B., Pithawalla, Y. B., and Naworal, J. D.: Carbohydrate pyrolysis mechanisms from isotopic labeling, Part 3. The Pyrolysis of D-glucose: formation of C-3 and C-4 carbonyl compounds and a cyclopentenedione isomer by electrocyclic fragmentation mechanisms, *J. Anal. Appl. Pyrol.*, 82, 42–69, 2008a.
- Paine, J. B., Pithawalla, Y. B., and Naworal, J. D.: Carbohydrate pyrolysis mechanisms from isotopic labeling Part 4. The pyrolysis Of D-glucose: the formation of furans, *J. Anal. Appl. Pyrol.*, 83, 37–63, 2008b.
- Pankow, J. F., Luo, W. T., Isabelle, L. M., Bender, D. A., and Baker, R. J.: Determination of a wide range of volatile organic compounds in ambient air using multisorbent adsorption/thermal desorption and gas chromatography mass spectrometry, *Anal. Chem.*, 70, 5213–5221, doi:10.1021/Ac980481t, 1998.
- Pankow, J. F., Luo, W., Melnychenko, A. N., Barsanti, K. C., Isabelle, L. M., Chen, C., Guenther, A. B., and Rosenstiel, T. N.: Volatilizable Biogenic Organic Compounds (VBOCs) with two dimensional Gas Chromatography-Time of Flight Mass Spectrometry (GC×GC-TOFMS): sampling methods, VBOC complexity, and chromatographic retention data, *Atmos. Meas. Tech.*, 5, 345–361, doi:10.5194/amt-5-345-2012, 2012.
- Patwardhan, P. R., Satrio, J. A., Brown, R. C., and Shanks, B. H.: Influence of inorganic salts on the primary pyrolysis products of cellulose, *Bioresource Technol.*, 101, 4646–4655, doi:10.1016/J.Biortech.2010.01.112, 2010.
- Petters, M. D., Parsons, M. T., Prenni, A. J., DeMott, P. J., Kreidenweis, S. M., Carrico, C. M., Sullivan, A. P., McMeeking, G. R., Levin, E., Wold, C. E., Collett, J. L., and Moosmuller, H.: Ice nuclei emissions from biomass burning, *J. Geophys. Res.-Atmos.*, 114, D07209, doi:10.1029/2008jd011532, 2009.
- Pollmann, J., Ortega, J., and Helmig, D.: Analysis of atmospheric sesquiterpenes: sampling losses and mitigation of ozone interferences, *Environ. Sci. Technol.*, 39, 9620–9629, 2005.

23274

- Poschl, U.: Atmospheric aerosols: composition, transformation, climate and health effects, *Angew. Chem. Int. Edit.*, 44, 7520–7540, doi:10.1002/anie.200501122, 2005.
- Presto, A. A., Miracolo, M. A., Donahue, N. M., and Robinson, A. L.: Secondary organic aerosol formation from high-NO_x photo-oxidation of low volatility precursors: *n*-alkanes, *Environ. Sci. Technol.*, 44, 2029–2034, 2010.
- Reid, J. S., Koppmann, R., Eck, T. F., and Eleuterio, D. P.: A review of biomass burning emissions part II: intensive physical properties of biomass burning particles, *Atmos. Chem. Phys.*, 5, 799–825, doi:10.5194/acp-5-799-2005, 2005.
- Saiz-Jimenez, C. and De Leeuw, J. W.: Lignin pyrolysis products: their structures and their significance as biomarkers *Org. Geochem.*, 10, 869–876, 1986.
- Saxena, P., Hildemann, L. M., McMurry, P. H., and Seinfeld, J. H.: Organics alter hygroscopic behavior of atmospheric particles, *J. Geophys. Res.-Atmos.*, 100, 18755–18770, 1995.
- Schauer, J. J., Kleeman, M. J., Cass, G. R., and Simoneit, B. R. T.: Measurement of emissions from air pollution sources. 3. C-1–C-29 organic compounds from fireplace combustion of wood, *Environ. Sci. Technol.*, 35, 1716–1728, 2001.
- Seinfeld, J. H. and Pankow, J. F.: Organic atmospheric particulate material, *Annu. Rev. Phys. Chem.*, 54, 121–140, doi:10.1146/annurev.physchem.54.011002.103756, 2003.
- Shafizadeh, F.: Introduction to pyrolysis of biomass, *J. Anal. Appl. Pyrol.*, 3, 283–305, 1982.
- Simpson, I. J., Akagi, S. K., Barletta, B., Blake, N. J., Choi, Y., Diskin, G. S., Fried, A., Fuenberg, H. E., Meinardi, S., Rowland, F. S., Vay, S. A., Weinheimer, A. J., Wennberg, P. O., Wiebring, P., Wisthaler, A., Yang, M., Yokelson, R. J., and Blake, D. R.: Boreal forest fire emissions in fresh Canadian smoke plumes: C₁–C₁₀ volatile organic compounds (VOCs), CO₂, CO, NO₂, NO, HCN and CH₃CN, *Atmos. Chem. Phys.*, 11, 6445–6463, doi:10.5194/acp-11-6445-2011, 2011.
- Smith, J. D., Sio, V., Yu, L., Zhang, Q., and Anastasio, C.: Secondary organic aerosol production from aqueous reactions of atmospheric phenols with an organic triplet excited state, *Environ. Sci. Technol.*, 48, 1049–1057, doi:10.1021/Es4045715, 2014.
- Sojak, L., Hrivnak, J., Majer, P., and Janak, J.: Capillary gas-chromatography of linear alkenes on squalane, *Anal. Chem.*, 45, 293–302, 1973.
- Sojak, L., Kralovicova, E., Ostrovsky, I., and Leclercq, P. A.: Retention behavior of conjugated and isolated normal-alkadienes – identification of normal-nonadiene and normal-decadiene by capillary gas-chromatography using structure retention correlations and mass-spectrometry, *J. Chromatogr.*, 292, 241–261, 1984.

23275

- Stein, S. E.: Retention indices, in: NIST Chemistry WebBook, NIST Standard Reference Database Number 69, edited by: Linstrom, P. J. and Mallard, W. G., National Institute of Standards and Technology, Gaithersburg, MD, 20899, available at: <http://webbook.nist.gov>, last access: 2013.
- Stockwell, C. E., Yokelson, R. J., Kreidenweis, S. M., Robinson, A. L., DeMott, P. J., Sullivan, R. C., Reardon, J., Ryan, K. C., Griffith, D. W. T., and Stevens, L.: Trace gas emissions from combustion of peat, crop residue, biofuels, grasses, and other fuels: configuration and FTIR component of the fourth Fire Lab at Missoula Experiment (FLAME-4), *Atmos. Chem. Phys. Discuss.*, 14, 10061–10134, doi:10.5194/acpd-14-10061-2014, 2014.
- Stolle, A., Ondruschka, B., and Hopf, H.: Thermal rearrangements of monoterpenes and monoterpenoids, *Helv. Chim. Acta*, 92, 1673–1719, 2009.
- Streets, D. G., Yarber, K. F., Woo, J. H., and Carmichael, G. R.: Biomass burning in Asia: annual and seasonal estimates and atmospheric emissions, *Global Biogeochem. Cy.*, 17, 1099, doi:10.1029/2003GB002040, 2003.
- Strollo, C. M. and Ziemann, P. J.: Products and mechanism of secondary organic aerosol formation from the reaction of 3-methylfuran with OH radicals in the presence of NO_x, *Atmos. Environ.*, 77, 534–543, 2013.
- Surratt, J. D., Murphy, S. M., Kroll, J. H., Ng, N. L., Hildebrandt, L., Sorooshian, A., Szmigielski, R., Vermeylen, R., Maenhaut, W., Claeys, M., Flagan, R. C., and Seinfeld, J. H.: Chemical composition of secondary organic aerosol formed from the photooxidation of isoprene, *J. Phys. Chem. A*, 110, 9665–9690, 2006.
- Tong, H. Y. and Karasek, F. W.: Flame ionization detector response factors for compound classes in quantitative-analysis of complex organic mixtures, *Anal. Chem.*, 56, 2124–2128, 1984.
- Vakkari, V., Kerminen, V. M., Beukes, J. P., Tiitta, P., van Zyl, P. G., Josipovic, M., Venter, A. D., Jaars, K., Worsnop, D. R., Kulmala, M., and Laakso, L.: Rapid changes in biomass burning aerosols by atmospheric oxidation, *Geophys. Res. Lett.*, 41, 2644–2651, doi:10.1002/2014gl059396, 2014.
- van der Werf, G. R., Randerson, J. T., Giglio, L., Collatz, G. J., Mu, M., Kasibhatla, P. S., Morton, D. C., DeFries, R. S., Jin, Y., and van Leeuwen, T. T.: Global fire emissions and the contribution of deforestation, savanna, forest, agricultural, and peat fires (1997–2009), *Atmos. Chem. Phys.*, 10, 11707–11735, doi:10.5194/acp-10-11707-2010, 2010.

23276

- Veblen, T. T., Kitzberger, T., and Donnegan, J.: Climatic and human influences on fire regimes in ponderosa pine forests in the Colorado Front Range, *Ecol. Appl.*, 10, 1178–1195, 2000.
- von Rudloff, E.: Seasonal variation in the terpenes of the foliage of black spruce, *Phytochemistry*, 14, 1695–1699, 1975.
- 5 Wade, D. D., Brock, B. L., Brose, P. H., Grace, J. B., Hoch, G. A., and Patterson, W. A.: Fire in Eastern Ecosystems, in: *Wildland Fire in Ecosystems: Effects of Fire on Flora*. Gen. Tech. Rep. RMRS-GTR-42-vol. 2, edited by: Brown, J. K. and Smith, J. K., US Department of Agriculture, Forest Service, Rocky Mountain Research Station, Ogden, UT, 53–96, 2000.
- Wang, Q., Jacob, D. J., Fisher, J. A., Mao, J., Leibensperger, E. M., Carouge, C. C., Le Sager, P.,
10 Kondo, Y., Jimenez, J. L., Cubison, M. J., and Doherty, S. J.: Sources of carbonaceous aerosols and deposited black carbon in the Arctic in winter-spring: implications for radiative forcing, *Atmos. Chem. Phys.*, 11, 12453–12473, doi:10.5194/acp-11-12453-2011, 2011.
- Ward, D. E.: Factors influencing the emissions of gases and particulate matter from biomass burning, in: *Fire in the Tropical Biota: Ecosystem Processes and Global Challenges*, edited by: Goldammer, J. G., Springer-Verlag, Berlin, Germany, 418–436, 1990.
- 15 Warneke, C., Roberts, J. M., Veres, P., Gilman, J., Kuster, W. C., Burling, I., Yokelson, R., and de Gouw, J. A.: VOC identification and inter-comparison from laboratory biomass burning using PTR-MS and PIT-MS, *Int. J. Mass. Spectrom.*, 303, 6–14, doi:10.1016/j.ijms.2010.12.002, 2011.
- 20 Wiedinmyer, C., Akagi, S. K., Yokelson, R. J., Emmons, L. K., Al-Saadi, J. A., Orlando, J. J., and Soja, A. J.: The Fire INventory from NCAR (FINN): a high resolution global model to estimate the emissions from open burning, *Geosci. Model Dev.*, 4, 625–641, doi:10.5194/gmd-4-625-2011, 2011.
- Wigder, N. L., Jaffe, D. A., and Saketa, F. A.: Ozone and particulate matter enhancements
25 from regional wildfires observed at Mount Bachelor during 2004–2011, *Atmos. Environ.*, 75, 24–31, 2013.
- Yee, L. D., Kautzman, K. E., Loza, C. L., Schilling, K. A., Coggon, M. M., Chhabra, P. S., Chan, M. N., Chan, A. W. H., Hersey, S. P., Crounse, J. D., Wennberg, P. O., Flagan, R. C., and Seinfeld, J. H.: Secondary organic aerosol formation from biomass burning intermediates: phenol and methoxyphenols, *Atmos. Chem. Phys.*, 13, 8019–8043, doi:10.5194/acp-13-8019-2013, 2013.
- 30 Yokelson, R. J., Griffith, D. W. T., and Ward, D. E.: Open-path Fourier transform infrared studies of large-scale laboratory biomass fires, *J. Geophys. Res.-Atmos.*, 101, 21067–21080, 1996.

23277

- Yokelson, R. J., Goode, J. G., Ward, D. E., Susott, R. A., Babbitt, R. E., Wade, D. D., Bertschi, I., Griffith, D. W. T., and Hao, W. M.: Emissions of formaldehyde, acetic acid, methanol, and other trace gases from biomass fires in North Carolina measured by airborne Fourier transform infrared spectroscopy, *J. Geophys. Res.*, 104, 30109–30125, 1999.
- 5 Yokelson, R. J., Bertschi, I. T., Christian, T. J., Hobbs, P. V., Ward, D. E., and Hao, W. M.: Trace gas measurements in nascent, aged, and cloud-processed smoke from African savanna fires by airborne Fourier transform infrared spectroscopy (AFTIR), *J. Geophys. Res.-Atmos.*, 108, 8478, doi:10.1029/2002jd002322, 2003.
- Yokelson, R. J., Crounse, J. D., DeCarlo, P. F., Karl, T., Urbanski, S., Atlas, E., Campos, T.,
10 Shinozuka, Y., Kapustin, V., Clarke, A. D., Weinheimer, A., Knapp, D. J., Montzka, D. D., Holloway, J., Weibring, P., Flocke, F., Zheng, W., Toohey, D., Wennberg, P. O., Wiedinmyer, C., Mauldin, L., Fried, A., Richter, D., Walega, J., Jimenez, J. L., Adachi, K., Buseck, P. R., Hall, S. R., and Shetter, R.: Emissions from biomass burning in the Yucatan, *Atmos. Chem. Phys.*, 9, 5785–5812, doi:10.5194/acp-9-5785-2009, 2009.
- 15 Yokelson, R. J., Burling, I. R., Gilman, J. B., Warneke, C., Stockwell, C. E., de Gouw, J., Akagi, S. K., Urbanski, S. P., Veres, P., Roberts, J. M., Kuster, W. C., Reardon, J., Griffith, D. W. T., Johnson, T. J., Hosseini, S., Miller, J. W., Cocker III, D. R., Jung, H., and Weise, D. R.: Coupling field and laboratory measurements to estimate the emission factors of identified and unidentified trace gases for prescribed fires, *Atmos. Chem. Phys.*, 13, 89–116, doi:10.5194/acp-13-89-2013, 2013.
- 20 Ziemann, P. J.: Effects of molecular structure on the chemistry of aerosol formation from the OH-radical-initiated oxidation of alkanes and alkenes, *Int. Rev. Phys. Chem.*, 30, 161–195, 2011.
- Ziemann, P. J. and Atkinson, R.: Kinetics, products, and mechanisms of secondary organic aerosol formation, *Chem. Soc. Rev.*, 41, 6582–6605, 2012.
- 25

23278

Table 1. GC × GC/TOFMS conditions.

	Setting
GC injector	225 °C, 10 : 1 split
Column Flow	1.20 mL min ⁻¹
Primary Column	DB-VRX, 30 m, 0.25 mm I.D., 1.4 µm film (Agilent, Santa Clara, CA)
Primary Oven Program	45 °C for 5 min, 4 °C min ⁻¹ to 235 °C, 235 °C for 2.5 min
GC × GC Modulation	5 s period, 1.10 s hot pulse
GC × GC Modulator	Trapped with cold gas from LN2, then hot pulse at 25 °C above primary oven for release to secondary column
Secondary Column	Stabilwax, 1.5 m, 0.25 mm I.D., 0.5 µm film (Restek, Bellefonte, PA)
Secondary Oven	15 °C above primary oven
MS Source	200 °C, Electron impact, 70 eV
MS Detector	1500 V
MS Data Acquisition	227 spectra s ⁻¹ , 34–500 amu

23279

Table 2. Volatilizable compounds observed in the filter-desorption samples. Compounds in bold were positively identified by comparison with commercial standards. No compounds were observed in the wiregrass sample.

Compound	Formula	Primary RT (s)	Secondary RT (s)	Black Spruce	Pond. Pine	Cutgrass	Rice Straw	Ind. Peat
Eucalyptol	C ₁₀ H ₁₈ O	1479.53	1.36	x	–	–	–	–
C ₁₀ H ₁₈ O isomer	C ₁₀ H ₁₈ O	1784.44	2.275	x	–	–	–	–
4-Ethyl Phenol	C ₈ H ₁₀ O	1794.43	2.583	x	x	–	x	–
Borneol	C ₁₀ H ₁₈ O	1819.42	2.763	x	–	–	–	–
2,3-Dimethyl phenol	C ₈ H ₁₀ O	1839.42	0.304	–	–	–	x	–
p-Methylguaiacol	C ₉ H ₁₀ O ₂	1894.4	4.937	x	x	–	–	x
C ₈ H ₈ O isomer (?)	C ₈ H ₈ O	1919.39	4.268	x	x	–	x	–
Fenchyl acetate	C ₁₂ H ₂₀ O ₂	1954.38	1.5	x	–	–	–	–
4-Ethylguaiacol	C ₉ H ₁₂ O ₂	2084.34	4.316	–	x	–	–	–
1H-Pyrrole, 1-phenyl-	C ₁₀ H ₉ N	2089.34	3.296	–	x	–	–	–
4-Vinyl guaiacol	C ₉ H ₁₀ O ₂	2169.31	0.845	x	x	–	x	–
p-Propylguaiacol	C ₁₀ H ₁₄ O ₂	2264.28	3.903	–	x	–	–	–
1,13-Tetradecadiene	C ₁₄ H ₂₆	2269.28	1.17	–	x	–	–	–
1-Tetradecene	C ₁₄ H ₂₆	2284.28	1.118	x	x	–	x	x
Tetradecane	C ₁₄ H ₂₈	2299.27	1.06	x	x	–	x	x
Naphthalene, 2-ethenyl-	C ₁₂ H ₁₀	2439.23	3.137	–	x	–	–	–
Isoeugenol, c&t	C ₁₀ H ₁₂ O ₂	2449.22	0.119	–	x	–	–	–
Benzene, octyl-	C ₁₄ H ₂₂	2454.22	1.514	–	–	–	–	x
1-Pentadecene	C ₁₅ H ₃₀	2479.21	1.126	x	x	–	–	x
Pentadecane	C ₁₅ H ₃₂	2489.21	1.074	x	x	–	x	x
C ₁₅ H ₂₄ isomer	C ₁₅ H ₂₄	2509.2	1.474	–	x	–	–	–
C ₁₅ H ₂₄ isomer	C ₁₅ H ₂₄	2584.18	1.434	x	–	–	–	–
C ₁₇ H ₃₀ isomer	C ₁₇ H ₃₀	2584.18	1.914	–	–	–	–	x
Dibenzofuran	C ₁₂ H ₈ O	2614.17	3.599	–	x	x	–	–
Benzene, nonyl-	C ₁₅ H ₂₄	2649.16	1.509	–	–	–	–	x
1-Hexadecene	C ₁₆ H ₃₂	2664.15	1.135	–	–	–	–	x
Hexadecane	C ₁₆ H ₃₄	2674.15	1.082	x	x	–	–	x
Naphthalene, trimethyl-	C ₁₃ H ₁₄	2759.12	2.776	–	x	–	–	x
1-Heptadecene	C ₁₆ H ₃₂	2834.1	1.153	–	–	–	–	x
Heptadecane	C ₁₆ H ₃₄	2844.1	1.096	–	–	–	–	x
Octadecane	C ₁₈ H ₃₆	2884.08	2.31	–	–	–	–	x
1-Octadecene	C ₁₈ H ₃₆	2999.05	1.166	–	–	–	–	x
Octadecane	C ₁₈ H ₃₈	3009.04	1.113	–	–	–	–	x
Phenanthrene/Anthracene	C ₁₄ H ₁₀	3094.02	4.554	–	x	x	–	–

23280

Category	Black Spruce	Pond. Pine	Cutgrass	Wiregrass	Rice Straw	Ind. Peat
Aromatic Hydrocarbons ^a	0.63	0.77	0.32	0.04	0.18	1.09
Phenols ^b	0.04	0.16	0.04	0.02	0.09	0.15
Aliphatic Hydrocarbons ^c	0.05	0.1	0.001	0	0.03	0.55
Oxygenated Aliphatics ^d	0.06	0.1	0.01	0.02	0.05	0.07
Terpenes ^e	0.51	0.42	0.002	0.001	0.01	0.008
Furans ^f	0.08	0.13	0.01	0.04	0.06	0.1
Total Potential SOA	1.4	1.7	0.38	0.12	0.42	1.97
Typical POA EF ^g	9.92	28.16	4.16	5.6	9.92	9.92
OA Enhancement Ratio	1.14	1.06	1.09	1.02	1.04	1.20

Assumed SOA Yields:
^a Benzene derivatives: 0.3 (Ng et al., 2007), naphthalene derivatives: 0.7 (Chan et al., 2009).
^b 0.25 (Yee et al., 2013).
^c Alkanes: C_n -dependent values from Lim and Ziemann (2009), alkenes: C_n -dependent values from Matsunaga et al. (2009).
^d 0.05 based on methacrolein and methyl vinyl ketone (Liu et al., 2012).
^e Reported MT isomer-specific yields from Lee et al. (2006) were used; yields for all other MT isomers assumed to be 0.15, SQT yield estimated at 0.65.
^f 0.1 based on Ströckle and Ziemann (2013).
^g Fuel-specific "Organic Carbon" EFs reported in McMeeking et al. (2009) for BS, PP, WG, and RS; and the average OC EF from savannah and peatland fuels for CG and IP, respectively (Akagi et al., 2011). The OC EFs were scaled to OA by the factor of 1.6 based on measured BB OM/OC ratios (Aiken et al., 2008).

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emmission Factors (g kg ⁻¹)	Wiregrass	Rice Straw	Indonesian Peat
						Giant Cutgrass			
Burn and Fuel Characteristics									
Burn Number				156	144	148	151	153	154
MCE				0.933	0.927	0.925	0.970	0.942	0.832
Carbon (wt %)				50.5	51.11	44.84		42.07	59.71
Hydrogen (wt %)				6.37	6.64	6.1	6.32	5.68	5.01
Nitrogen (wt %)				0.66	1.09	2.03	0.61	1.3	2.28
Sulfur (wt %)				0.054	N/A	0.207	N/A	0.212	0.119
Ash (wt %)				3.8	1.5	2.3		7.7	3.8
Aromatic Hydrocarbons									
0 D.B.E. (of substituents)									
Benzene	C ₆ H ₆	454.861	1.672	0.55± 0.11	0.78± 0.14	0.27± 0.05	0.031 ± 0.008	0.14± 0.03	0.88± 0.18
Toluene	C ₇ H ₈	754.765	1.672	0.41± 0.08	0.41± 0.1	0.098± 0.02	0.028 ± 0.006	0.14± 0.03	0.90± 0.18
Ethylbenzene	C ₈ H ₁₀	1024.68	1.628	0.063± 0.031	0.080± 0.016	0.011 ± 0.002	(3.9 ± 1.7) × 10 ⁻³	0.19± 0.004	0.15± 0.03
m&p-Xylene	C ₈ H ₁₀	1064.67	1.619	0.13± 0.03	0.15± 0.03	0.012 ± 0.003	(6.6 ± 3.6) × 10 ⁻³	0.035 ± 0.007	0.35± 0.07
o-Xylene	C ₈ H ₁₀	1129.64	1.72	0.051 ± 0.01	0.055 ± 0.011	(3.1 ± 1.5) × 10 ⁻³	—	0.015 ± 0.003	0.18± 0.04
Benzene, isopropyl-	C ₉ H ₁₂	1199.62	1.544	(9.1 ± 1.8) × 10 ⁻³	(8.4 ± 1.7) × 10 ⁻³	(5.9 ± 1.4) × 10 ⁻⁴	—	(7.9 ± 1.6) × 10 ⁻⁴	(4.9 ± 1.3) × 10 ⁻³
Benzene, propyl-	C ₉ H ₁₂	1284.6	1.566	(9.3 ± 2.2) × 10 ⁻³	0.012 ± 0.002	—	—	(2.1 ± 0.6) × 10 ⁻³	0.044 ± 0.009
Benzene, 1,3,5-trimethyl-	C ₉ H ₁₂	1349.57	1.602	(4.8 ± 1.7) × 10 ⁻³	(7.8 ± 2.0) × 10 ⁻³	—	—	(2.3 ± 0.6) × 10 ⁻³	0.017 ± 0.006
Benzene, 1-ethyl-2-methyl-	C ₉ H ₁₂	1364.57	1.65	0.012 ± 0.002	0.015 ± 0.003	(6.7 ± 2.1) × 10 ⁻⁴	—	(2.9 ± 0.6) × 10 ⁻³	0.048 ± 0.01
Benzene, 1,2,4-trimethyl-	C ₉ H ₁₂	1419.55	1.65	0.012 ± 0.002	0.018 ± 0.004	(8.4 ± 2.5) × 10 ⁻⁴	(7.0 ± 3.7) × 10 ⁻⁴	(5.9 ± 1.2) × 10 ⁻³	0.076 ± 0.015
Benzene, 1,2,3-trimethyl-	C ₉ H ₁₂	1494.53	1.76	0.017 ± 0.003	0.024 ± 0.005	—	—	(3.1 ± 0.6) × 10 ⁻³	0.060 ± 0.012
Isobutylbenzene	C ₁₀ H ₁₄	1429.55	1.487	(2.3 ± 0.5) × 10 ⁻³	—	—	—	(6.1 ± 1.3) × 10 ⁻³	(5.5 ± 1.3) × 10 ⁻³
m-Cymene	C ₁₀ H ₁₄	1464.54	1.509	(7.7 ± 1.5) × 10 ⁻³	0.012 ± 0.002	—	—	(6.4 ± 1.2) × 10 ⁻⁴	(6.1 ± 1.2) × 10 ⁻³
p-Cymene	C ₁₀ H ₁₄	1474.53	1.514	0.039 ± 0.008	0.039 ± 0.008	—	—	(8.4 ± 2.6) × 10 ⁻⁴	0.023 ± 0.005
o-Cymene	C ₁₀ H ₁₄	1509.52	1.566	(1.4 ± 0.3) × 10 ⁻³	—	—	—	—	—
Benzene, 1,4-diethyl-	C ₁₀ H ₁₄	1534.52	1.527	(1.8 ± 0.9) × 10 ⁻³	(2.7 ± 1.3) × 10 ⁻³	—	—	(5.8 ± 2.9) × 10 ⁻⁴	—
Benzene, 1-methyl-3-propyl-	C ₁₀ H ₁₄	1544.51	1.527	(3.0 ± 0.6) × 10 ⁻³	(4.3 ± 0.9) × 10 ⁻³	—	—	(1.0 ± 0.2) × 10 ⁻³	0.015 ± 0.003
Benzene, 1-methyl-4-propyl-	C ₁₀ H ₁₄	1554.51	1.536	(2.4 ± 0.5) × 10 ⁻³	(3.1 ± 0.6) × 10 ⁻³	—	—	(6.7 ± 1.3) × 10 ⁻⁴	0.011 ± 0.002
Benzene, butyl-	C ₁₀ H ₁₄	1554.51	1.549	(6.6 ± 1.3) × 10 ⁻³	(9.2 ± 1.8) × 10 ⁻³	—	—	(1.2 ± 0.2) × 10 ⁻³	0.029 ± 0.006
Benzene, 5-ethyl-1,3-dimethyl-	C ₁₀ H ₁₄	1569.55	1.558	(3.2 ± 0.6) × 10 ⁻³	(3.7 ± 0.7) × 10 ⁻³	—	—	(1.1 ± 0.2) × 10 ⁻³	(9.7 ± 2.1) × 10 ⁻⁴
Benzene, 1-methyl-2-propyl-									

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
						Giant Cutgrass	Wiregrass		
Benzene, hexyl-	C ₁₂ H ₁₈	2029.36	1.518	(2.7 ± 1.4) × 10 ⁻³	(3.6 ± 1.8) × 10 ⁻³	–	–	(6.0 ± 3.7) × 10 ⁻⁴	0.019 ± 0.005
Benzene, (1,3-dimethylbutyl)-	C ₁₂ H ₁₈	2054.35	1.553	–	(2.9 ± 1.7) × 10 ⁻³	–	–	–	0.011 ± 0.005
Benzene, heptyl- 1 D.B.E. (of substituents)	C ₁₃ H ₂₀	2249.29	1.509	–	–	–	–	–	(9.3 ± 5.0) × 10 ⁻³
Styrene	C ₈ H ₈	1119.65	2.094	0.098 ± 0.02	0.14 ± 0.03	0.036 ± 0.007	(6.3 ± 1.3) × 10 ⁻³	0.028 ± 0.006	0.084 ± 0.017
Benzene, 2-propenyl-	C ₉ H ₁₀	1259.6	1.826	–	(6.4 ± 3.2) × 10 ⁻³	–	–	(1.3 ± 0.6) × 10 ⁻³	0.012 ± 0.006
α-Methylstyrene	C ₉ H ₁₀	1364.57	1.914	0.013 ± 0.003	0.016 ± 0.003	(1.2 ± 0.3) × 10 ⁻³	–	(2.3 ± 0.5) × 10 ⁻³	(6.5 ± 2.7) × 10 ⁻³
cis-1-Propenylbenzene	C ₉ H ₁₀	1364.56	1.892	(3.7 ± 0.8) × 10 ⁻³	(5.0 ± 1.0) × 10 ⁻³	–	–	(1.2 ± 0.2) × 10 ⁻³	(6.2 ± 2.6) × 10 ⁻³
Benzene, 1-ethenyl-3-methyl-	C ₉ H ₁₀	1414.55	1.954	0.045 ± 0.022	0.063 ± 0.031	(6.0 ± 3.0) × 10 ⁻³	(1.9 ± 1.0) × 10 ⁻³	(9.9 ± 5.0) × 10 ⁻³	0.044 ± 0.022
4-methyl styrene	C ₉ H ₁₀	1424.55	1.949	0.011 ± 0.005	0.011 ± 0.006	(1.6 ± 0.8) × 10 ⁻³	–	(2.4 ± 1.2) × 10 ⁻³	–
Benzene, 1-propenyl, trans	C ₉ H ₁₀	1494.53	2.02	(7.5 ± 1.5) × 10 ⁻³	0.011 ± 0.002	(1.3 ± 0.3) × 10 ⁻³	–	(2.4 ± 0.5) × 10 ⁻³	0.020 ± 0.004
Indane	C ₉ H ₁₀	1509.52	1.91	(6.0 ± 3.0) × 10 ⁻³	0.011 ± 0.006	(9.1 ± 4.6) × 10 ⁻⁴	–	(2.3 ± 1.2) × 10 ⁻³	0.026 ± 0.013
o-Isopropenyltoluene	C ₁₀ H ₁₂	1439.55	1.628	(2.2 ± 0.4) × 10 ⁻³	(3.9 ± 0.8) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1519.52	1.769	(2.8 ± 1.4) × 10 ⁻³	(4.2 ± 2.1) × 10 ⁻³	–	–	(8.9 ± 4.5) × 10 ⁻⁴	(7.7 ± 3.9) × 10 ⁻³
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1554.51	1.791	(2.8 ± 1.4) × 10 ⁻³	–	–	–	(6.5 ± 3.2) × 10 ⁻⁴	–
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1609.49	1.822	(2.3 ± 1.1) × 10 ⁻³	–	–	–	(6.5 ± 3.2) × 10 ⁻⁴	(7.3 ± 3.7) × 10 ⁻³
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1614.49	1.782	–	(4.0 ± 2.0) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1624.49	1.822	(6.5 ± 3.2) × 10 ⁻³	0.012 ± 0.006	–	–	(1.7 ± 0.8) × 10 ⁻³	–
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1634.48	1.857	(4.5 ± 2.2) × 10 ⁻³	(7.9 ± 3.9) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1639.48	1.764	–	–	–	–	–	0.011 ± 0.005
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1649.48	1.826	0.024 ± 0.012	0.024 ± 0.012	–	–	(1.5 ± 0.8) × 10 ⁻³	0.019 ± 0.01
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1659.48	1.866	(2.4 ± 1.2) × 10 ⁻³	(3.3 ± 1.7) × 10 ⁻³	–	–	(7.3 ± 3.7) × 10 ⁻⁴	–
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1679.47	1.874	–	–	–	–	(7.4 ± 3.7) × 10 ⁻⁴	–
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1689.47	1.866	–	–	–	–	(6.5 ± 3.2) × 10 ⁻⁴	–
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1734.45	1.901	(3.0 ± 1.5) × 10 ⁻³	(3.4 ± 1.7) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1759.44	1.923	(3.3 ± 1.6) × 10 ⁻³	(4.6 ± 2.3) × 10 ⁻³	–	–	(1.4 ± 0.7) × 10 ⁻³	(7.9 ± 3.9) × 10 ⁻³
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1779.44	1.835	(2.1 ± 1.0) × 10 ⁻³	(3.6 ± 1.8) × 10 ⁻³	–	–	(8.7 ± 4.3) × 10 ⁻⁴	0.011 ± 0.005
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1804.43	1.896	–	(3.9 ± 2.0) × 10 ⁻³	–	–	(8.8 ± 4.4) × 10 ⁻⁴	0.014 ± 0.007
C ₁₀ H ₁₂ isomer	C ₁₀ H ₁₂	1829.42	1.98	–	(3.0 ± 1.5) × 10 ⁻³	–	–	–	(8.5 ± 4.3) × 10 ⁻³
C ₁₁ H ₁₄ isomer	C ₁₁ H ₁₄	1769.44	1.729	(4.3 ± 2.1) × 10 ⁻³	–	–	–	–	–
C ₁₁ H ₁₄ isomer	C ₁₁ H ₁₄	1909.4	1.769	–	(4.1 ± 2.1) × 10 ⁻³	–	–	–	0.011 ± 0.008
C ₁₁ H ₁₄ isomer	C ₁₁ H ₁₄	2584.18	1.91	–	–	–	–	–	0.018 ± 0.009
2 D.B.E. (of substituents)									
Phenylacetylene	C ₈ H ₆	1064.67	3.089	0.027 ± 0.005	0.032 ± 0.006	0.026 ± 0.005	(2.9 ± 0.7) × 10 ⁻³	(5.5 ± 1.1) × 10 ⁻³	–
Benzene, 1-ethynyl-2-methyl-	C ₉ H ₈	1369.57	2.715	(4.1 ± 2.0) × 10 ⁻³	(5.0 ± 2.5) × 10 ⁻³	(1.4 ± 0.7) × 10 ⁻³	–	(4.0 ± 2.0) × 10 ⁻⁴	–
Indene	C ₉ H ₈	1544.51	2.429	0.052 ± 0.026	0.068 ± 0.034	0.030 ± 0.015	(2.8 ± 1.4) × 10 ⁻³	0.014 ± 0.007	0.028 ± 0.014
C ₁₀ H ₁₀ isomer	C ₁₀ H ₁₀	1634.48	2.103	(2.2 ± 1.1) × 10 ⁻³	(2.8 ± 1.4) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₀ isomer	C ₁₀ H ₁₀	1714.46	2.268	(2.8 ± 1.4) × 10 ⁻³	(3.4 ± 1.7) × 10 ⁻³	–	–	(5.0 ± 2.5) × 10 ⁻⁴	–
C ₁₀ H ₁₀ isomer	C ₁₀ H ₁₀	1814.43	2.248	0.013 ± 0.006	0.020 ± 0.01	(3.4 ± 1.7) × 10 ⁻³	(1.2 ± 0.6) × 10 ⁻³	(5.9 ± 3.0) × 10 ⁻³	0.020 ± 0.01
C ₁₀ H ₁₀ isomer	C ₁₀ H ₁₀	1829.42	2.319	(8.7 ± 4.3) × 10 ⁻³	0.016 ± 0.008	(2.0 ± 1.0) × 10 ⁻³	–	(4.9 ± 2.4) × 10 ⁻³	0.020 ± 0.01
C ₁₀ H ₁₀ isomer	C ₁₀ H ₁₀	1839.42	2.341	(4.0 ± 2.0) × 10 ⁻³	(5.0 ± 2.5) × 10 ⁻³	(6.2 ± 3.1) × 10 ⁻⁴	–	(1.2 ± 0.6) × 10 ⁻³	–
C ₁₁ H ₁₂ isomer	C ₁₁ H ₁₂	1869.41	1.993	–	–	–	–	(4.5 ± 2.2) × 10 ⁻⁴	–
C ₁₁ H ₁₂ isomer	C ₁₁ H ₁₂	2024.36	2.178	–	–	–	–	(5.8 ± 2.9) × 10 ⁻⁴	–
C ₁₁ H ₁₂ isomer	C ₁₁ H ₁₂	2064.35	2.13	(1.7 ± 0.9) × 10 ⁻³	(2.5 ± 1.3) × 10 ⁻³	–	–	(9.2 ± 4.6) × 10 ⁻⁴	(6.7 ± 3.3) × 10 ⁻³
C ₁₁ H ₁₂ isomer	C ₁₁ H ₁₂	2079.34	2.196	(2.6 ± 1.3) × 10 ⁻³	(4.5 ± 2.2) × 10 ⁻³	–	–	(1.6 ± 0.8) × 10 ⁻³	0.010 ± 0.005
C ₁₁ H ₁₂ isomer	C ₁₁ H ₁₂	2089.34	2.248	(2.9 ± 1.4) × 10 ⁻³	(5.0 ± 2.5) × 10 ⁻³	–	–	(1.7 ± 0.9) × 10 ⁻³	–
C ₁₁ H ₁₂ isomer	C ₁₁ H ₁₂	2094.34	2.226	–	–	–	–	–	0.010 ± 0.005

23283

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
						Giant Cutgrass	Wiregrass		
PAHs (and related)									
Naphthalene	C ₁₀ H ₈	1909.4	2.952	0.083 ± 0.017	0.089 ± 0.018	0.070 ± 0.014	(4.8 ± 1.0) × 10 ⁻³	0.026 ± 0.005	0.046 ± 0.009
Naphthalene, 2-methyl-	C ₁₁ H ₁₀	2164.31	2.741	0.014 ± 0.003	0.016 ± 0.003	(5.5 ± 1.1) × 10 ⁻³	(2.4 ± 0.7) × 10 ⁻³	(6.9 ± 1.4) × 10 ⁻³	0.035 ± 0.007
Naphthalene, 1-methyl-	C ₁₁ H ₁₀	2199.3	2.847	0.013 ± 0.003	0.016 ± 0.003	(5.0 ± 1.0) × 10 ⁻³	–	(5.5 ± 1.1) × 10 ⁻³	0.034 ± 0.007
Biphenyl	C ₁₂ H ₁₀	2314.27	2.952	(6.4 ± 2.3) × 10 ⁻³	(5.9 ± 2.8) × 10 ⁻³	(3.3 ± 0.8) × 10 ⁻³	–	(2.3 ± 0.6) × 10 ⁻³	0.021 ± 0.008
Naphthalene, 1-ethyl-	C ₁₂ H ₁₂	2364.25	2.596	(5.6 ± 5.5) × 10 ⁻³	–	–	–	(1.5 ± 1.4) × 10 ⁻³	–
Naphthalene, 1,6-dimethyl-	C ₁₂ H ₁₂	2429.23	2.662	–	–	–	–	(1.5 ± 1.4) × 10 ⁻³	–
Naphthalene, 1,3-dimethyl-	C ₁₂ H ₁₂	2439.23	2.666	(5.6 ± 5.5) × 10 ⁻³	(6.5 ± 6.6) × 10 ⁻³	–	–	(2.0 ± 1.4) × 10 ⁻³	0.047 ± 0.023
Acenaphthylene	C ₁₂ H ₈	2494.21	3.744	0.011 ± 0.002	0.012 ± 0.002	0.017 ± 0.003	(3.2 ± 0.9) × 10 ⁻³	(3.6 ± 0.7) × 10 ⁻³	–
Other									
4-Phenylbut-3-ene-1-yne	C ₁₀ H ₈	1844.42	2.886	(3.4 ± 1.7) × 10 ⁻³	(5.3 ± 2.7) × 10 ⁻³	(1.1 ± 0.6) × 10 ⁻³	–	(1.3 ± 0.6) × 10 ⁻³	–
Oxygenated Aromatic Compounds									
Alcohols									
Phenol	C ₆ H ₆ O	1334.58	3.538	0.13 ± 0.03	0.48 ± 0.1	0.15 ± 0.03	0.057 ± 0.011	0.26 ± 0.05	0.47 ± 0.09
Phenol, 2-methyl	C ₇ H ₈ O	1524.52	3.56	0.021 ± 0.006	0.050 ± 0.01	0.015 ± 0.003	0.011 ± 0.003	0.043 ± 0.009	0.095 ± 0.02
Phenol, 3 + 4-methyl o-Guaiacol	C ₇ H ₈ O	1579.5	0.959	0.019 ± 0.004	0.043 ± 0.009	0.010 ± 0.002	0.012 ± 0.002	0.027 ± 0.005	–
2,5-dimethyl phenol	C ₇ H ₈ O ₂	1644.48	1.065	0.013 ± 0.003	0.055 ± 0.011	–	0.020 ± 0.004	0.011 ± 0.002	0.079 ± 0.016
Phenol, 2,6-dimethyl-	C ₈ H ₁₀ O	1764.44	4.704	–	0.011 ± 0.002	–	–	(7.9 ± 2.8) × 10 ⁻³	–
	C ₈ H ₁₀ O	1679.47	1.584	–	–	–	–	(3.8 ± 1.9) × 10 ⁻³	–
Aldehydes									
Benzaldehyde	C ₇ H ₆ O	1309.59	3.802	0.060 ± 0.012	0.071 ± 0.014	0.034 ± 0.007	(4.4 ± 3.4) × 10 ⁻³	0.020 ± 0.004	0.030 ± 0.016
Salicylaldehyde	C ₇ H ₆ O ₂	1529.52	4.343	–	0.015 ± 0.003	(7.3 ± 1.5) × 10 ⁻³	–	(6.4 ± 1.3) × 10 ⁻³	–
Benzeneacetaldehyde	C ₈ H ₈ O	1519.52	3.85	(1.3 ± 0.6) × 10 ⁻³	(3.2 ± 5.5) × 10 ⁻³	–	–	(7.9 ± 11.8) × 10 ⁻⁴	–
Benzaldehyde, 2 + 3-methyl-	C ₈ H ₈ O	1604.49	3.247	0.020 ± 0.004	0.025 ± 0.005	(4.8 ± 1.0) × 10 ⁻³	–	(7.3 ± 1.5) × 10 ⁻³	–
Ketones									
Acetophenone	C ₈ H ₈ O	1594.5	3.533	(4.0 ± 0.8) × 10 ⁻³	(6.7 ± 1.3) × 10 ⁻³	(1.4 ± 0.3) × 10 ⁻³	(5.5 ± 5.0) × 10 ⁻⁴	(4.8 ± 1.0) × 10 ⁻³	0.011 ± 0.002
Acetophenone, 3'-methyl-	C ₉ H ₁₀ O	1864.41	3.115	–	–	–	–	(1.7 ± 0.3) × 10 ⁻³	–
1,2-Naphthalenedione	C ₁₀ H ₆ O ₂	1904.4	4.299	–	–	(6.7 ± 3.3) × 10 ⁻⁴	–	–	–
3,3-Dimethyl-1-indanone	C ₁₁ H ₁₂ O	2179.31	2.262	–	–	–	–	(1.7 ± 0.8) × 10 ⁻³	–
Furans									
Benzo fur an	C ₈ H ₆ O	1419.55	2.979	0.036 ± 0.007	0.045 ± 0.009	0.023 ± 0.005	(5.4 ± 1.1) × 10 ⁻³	0.019 ± 0.004	0.048 ± 0.01
Benzo fur an, 2,3-dihydro-	C ₈ H ₈ O	1624.49	2.913	–	–	–	–	(1.1 ± 0.6) × 10 ⁻³	–
Methyl benzo fur an isomer	C ₉ H ₈ O	1684.47	2.627	(4.1 ± 2.1) × 10 ⁻³	(6.0 ± 3.0) × 10 ⁻³	(1.7 ± 0.9) × 10 ⁻³	–	(3.0 ± 1.5) × 10 ⁻³	0.011 ± 0.006
Methyl benzo fur an isomer	C ₉ H ₈ O	1704.46	2.675	(8.1 ± 4.0) × 10 ⁻³	0.012 ± 0.006	(2.8 ± 1.4) × 10 ⁻³	(2.2 ± 1.1) × 10 ⁻³	(6.2 ± 3.1) × 10 ⁻³	0.023 ± 0.012
Methyl benzo fur an isomer	C ₉ H ₈ O	1714.46	2.565	(6.8 ± 3.4) × 10 ⁻³	0.013 ± 0.007	(2.2 ± 1.1) × 10 ⁻³	(2.1 ± 1.0) × 10 ⁻³	(5.3 ± 2.6) × 10 ⁻³	0.027 ± 0.014
Ethyl-benzo fur an isomer	C ₁₀ H ₁₀ O	1924.39	2.504	–	–	–	–	(1.4 ± 0.7) × 10 ⁻³	–
Ethyl-benzo fur an isomer	C ₁₀ H ₁₀ O	1939.39	2.341	–	–	–	–	(8.3 ± 4.2) × 10 ⁻⁴	–
Benzo fur an, -dimethyl- (isomer)	C ₁₀ H ₁₀ O	1944.38	2.336	–	(4.0 ± 2.0) × 10 ⁻³	–	–	(1.7 ± 0.9) × 10 ⁻³	0.013 ± 0.007
Benzo fur an, dimethyl- (isomer)	C ₁₀ H ₁₀ O	1974.37	2.385	(3.2 ± 1.6) × 10 ⁻³	(6.2 ± 3.1) × 10 ⁻³	–	–	(3.0 ± 1.5) × 10 ⁻³	0.016 ± 0.008
Ethyl-benzo fur an isomer	C ₁₀ H ₁₀ O	1989.37	2.394	–	–	–	–	(1.0 ± 0.5) × 10 ⁻³	–
Benzo fur an, 2-ethenyl-	C ₁₀ H ₈ O	2004.36	3.164	–	–	–	–	(10.0 ± 5.0) × 10 ⁻⁴	–

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
						Glant Cutgrass	Wiregrass		
Ethers and Esters									
Anisole	C ₇ H ₆ O	1189.63	2.468	(4.2 ± 0.9) × 10 ⁻³	(8.2 ± 1.6) × 10 ⁻³	(1.6 ± 0.3) × 10 ⁻³	(8.7 ± 4.9) × 10 ⁻⁴	(1.5 ± 0.3) × 10 ⁻³	–
4-methyl anisole	C ₉ H ₁₀ O	1474.53	2.244	(4.4 ± 2.2) × 10 ⁻³	0.011 ± 0.005	–	(1.9 ± 0.9) × 10 ⁻³	(1.7 ± 0.8) × 10 ⁻³	0.010 ± 0.005
Acetic acid, phenyl ester	C ₉ H ₈ O ₂	1564.51	3.252	–	–	–	–	(7.9 ± 3.9) × 10 ⁻⁴	–
2,3-Dimethylanisole	C ₉ H ₁₀ O	1694.46	2.011	–	–	–	–	–	(6.0 ± 3.2) × 10 ⁻³
4-ethyl anisole	C ₉ H ₁₀ O	1704.46	2.13	–	–	–	–	(5.3 ± 2.7) × 10 ⁻⁴	–
Benzoic acid, methyl ester	C ₉ H ₈ O ₂	1664.47	2.904	–	0.016 ± 0.008	–	–	–	(5.1 ± 2.5) × 10 ⁻³
Benzene, 1-ethenyl-4-methoxy-	C ₉ H ₁₀ O	1804.43	2.706	–	–	–	–	(5.5 ± 2.8) × 10 ⁻⁴	–
Estragole	C ₁₀ H ₁₂ O	1899.4	2.341	–	0.013 ± 0.003	–	–	–	–
Other									
1,3-Benzodioxole	C ₇ H ₆ O ₂	1419.55	3.238	(3.7 ± 1.8) × 10 ⁻³	–	(2.1 ± 1.0) × 10 ⁻³	–	(1.3 ± 0.6) × 10 ⁻³	–
Aliphatic Hydrocarbons									
0 D.B.E.									
Butane, 2-methyl-	C ₅ H ₁₂	159.955	0.898	(4.9 ± 1.0) × 10 ⁻³	–	–	–	(1.2 ± 0.4) × 10 ⁻³	0.036 ± 0.014
Pentane	C ₅ H ₁₂	174.95	0.906	0.032 ± 0.012	0.064 ± 0.015	–	–	(8.6 ± 3.4) × 10 ⁻³	0.33 ± 0.07
Pentane, 2-methyl-	C ₆ H ₁₄	249.926	0.937	(2.7 ± 1.6) × 10 ⁻³	(7.5 ± 2.5) × 10 ⁻³	–	–	(1.2 ± 0.5) × 10 ⁻³	0.049 ± 0.01
Pentane, 3-methyl-	C ₆ H ₁₄	269.92	0.95	–	(4.5 ± 1.9) × 10 ⁻³	–	–	–	(8.1 ± 5.1) × 10 ⁻³
Hexane	C ₆ H ₁₄	299.91	0.959	0.020 ± 0.004	0.048 ± 0.01	–	–	(3.7 ± 1.1) × 10 ⁻³	0.20 ± 0.04
Pentane, 2,4-dimethyl-	C ₇ H ₁₆	359.891	0.959	–	(4.4 ± 2.7) × 10 ⁻⁴	–	–	–	–
Hexane, 2-methyl-	C ₇ H ₁₆	449.862	0.972	(2.8 ± 0.6) × 10 ⁻⁴	(7.1 ± 2.8) × 10 ⁻⁴	–	(1.5 ± 0.3) × 10 ⁻⁴	(0.8 ± 0.2) × 10 ⁻⁴	(7.6 ± 1.6) × 10 ⁻³
Pentane, 2,3-dimethyl-	C ₇ H ₁₆	454.861	0.986	(8.6 ± 2.3) × 10 ⁻⁴	(1.7 ± 0.9) × 10 ⁻³	–	–	–	(7.5 ± 2.2) × 10 ⁻³
Hexane, 3-methyl-	C ₇ H ₁₆	469.856	0.981	–	–	–	–	–	0.010 ± 0.003
Heptane	C ₇ H ₁₆	534.835	0.986	0.016 ± 0.003	0.032 ± 0.006	–	(1.4 ± 0.3) × 10 ⁻³	(2.8 ± 0.6) × 10 ⁻³	0.19 ± 0.04
Pentane, 2,2,4-trimethyl-	C ₈ H ₁₈	509.843	0.968	(4.7 ± 2.3) × 10 ⁻³	–	(1.1 ± 0.5) × 10 ⁻³	(4.2 ± 2.1) × 10 ⁻³	–	–
Hexane, 2,5-dimethyl-	C ₈ H ₁₈	624.806	0.977	–	–	–	(2.7 ± 1.9) × 10 ⁻⁴	–	–
Hexane, 2,3-dimethyl-	C ₈ H ₁₈	709.779	0.994	–	–	–	–	(1.3 ± 0.3) × 10 ⁻⁴	–
Pentane, 2,3,3-trimethyl-	C ₈ H ₁₈	714.778	0.999	(1.6 ± 12.4) × 10 ⁻⁴	–	–	–	–	(5.2 ± 2.6) × 10 ⁻³
Heptane, 2-methyl-	C ₈ H ₁₈	724.774	0.986	–	–	–	–	–	0.034 ± 0.009
Heptane, 3-methyl-	C ₈ H ₁₈	744.768	0.99	–	–	–	–	–	(1.7 ± 3.8) × 10 ⁻³
Octane	C ₈ H ₁₈	824.742	0.994	(9.5 ± 2.3) × 10 ⁻³	0.027 ± 0.015	–	–	(1.5 ± 0.8) × 10 ⁻³	0.18 ± 0.04
Heptane, 2,6-dimethyl-	C ₉ H ₂₀	909.715	0.981	–	(1.6 ± 0.8) × 10 ⁻³	–	–	–	0.013 ± 0.007
Heptane, 2,3-dimethyl-	C ₉ H ₂₀	989.69	0.999	–	–	–	–	–	(6.3 ± 1.6) × 10 ⁻³
Octane, 2-methyl-	C ₉ H ₂₀	1014.68	0.99	–	–	–	–	–	(5.9 ± 3.9) × 10 ⁻³
Octane, 3-methyl-	C ₉ H ₂₀	1034.68	0.994	–	–	–	–	–	(5.7 ± 3.4) × 10 ⁻³
Nonane	C ₉ H ₂₀	1109.65	1.003	(6.2 ± 1.9) × 10 ⁻³	0.019 ± 0.004	–	–	(1.5 ± 0.7) × 10 ⁻³	0.15 ± 0.03
C ₁₀ H ₂₂ isomer	C ₁₀ H ₂₂	1209.62	0.994	–	(1.7 ± 1.0) × 10 ⁻³	–	–	(3.5 ± 2.1) × 10 ⁻⁴	–
C ₁₀ H ₂₂ isomer	C ₁₀ H ₂₂	1229.61	1.008	–	(3.6 ± 1.8) × 10 ⁻³	–	–	–	0.017 ± 0.008
C ₁₀ H ₂₂ isomer	C ₁₀ H ₂₂	1234.61	1.003	(1.9 ± 1.0) × 10 ⁻³	–	–	–	(3.5 ± 2.1) × 10 ⁻⁴	–
Nonane, 2-methyl-	C ₁₀ H ₂₂	1289.59	0.99	–	(1.1 ± 0.2) × 10 ⁻³	–	–	–	0.012 ± 0.002
Decane	C ₁₀ H ₂₂	1384.56	1.012	(5.4 ± 1.1) × 10 ⁻³	0.014 ± 0.003	–	–	(1.3 ± 0.3) × 10 ⁻³	0.14 ± 0.03
C ₁₀ H ₂₂ isomer	C ₁₀ H ₂₂	1449.54	0.994	–	(2.2 ± 1.1) × 10 ⁻³	–	–	(3.5 ± 2.1) × 10 ⁻⁴	–
C ₁₁ H ₂₄ isomer	C ₁₁ H ₂₄	1449.54	0.999	–	–	–	–	–	0.031 ± 0.016
C ₁₁ H ₂₄ isomer	C ₁₁ H ₂₄	1534.52	1.008	–	–	–	–	–	0.014 ± 0.008
C ₁₁ H ₂₄ isomer	C ₁₁ H ₂₄	1549.51	1.008	–	–	–	–	–	0.017 ± 0.008
Undecane	C ₁₁ H ₂₄	1634.48	1.025	(4.6 ± 3.1) × 10 ⁻³	0.025 ± 0.005	–	–	–	0.11 ± 0.02
C ₁₂ H ₂₆ isomer	C ₁₂ H ₂₆	1789.43	1.021	–	–	–	–	–	0.011 ± 0.01
Dodecane	C ₁₂ H ₂₆	1869.41	1.038	–	(4.5 ± 3.7) × 10 ⁻³	–	–	–	0.088 ± 0.018
C ₁₃ H ₂₈ isomer	C ₁₃ H ₂₈	1909.4	1.021	–	(1.8 ± 2.0) × 10 ⁻³	–	–	(3.8 ± 4.3) × 10 ⁻⁴	0.035 ± 0.018
Tridecane	C ₁₃ H ₂₈	2089.34	1.052	(2.8 ± 2.2) × 10 ⁻³	(3.9 ± 2.0) × 10 ⁻³	–	–	(8.4 ± 4.3) × 10 ⁻⁴	0.058 ± 0.012
Tetradecane	C ₁₄ H ₃₀	2299.27	1.06	–	–	–	–	(4.5 ± 2.2) × 10 ⁻⁴	0.026 ± 0.005

23285

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
C ₁₆ H ₃₂ isomer	C ₁₆ H ₃₂	2259.28	1.03	—	—	—	—	—	0.019 ± 0.01
C ₁₆ H ₃₂ isomer	C ₁₆ H ₃₂	2424.23	1.038	—	—	—	—	—	0.016 ± 0.008
Pentadecane	C ₁₅ H ₃₂	2489.21	1.074	—	—	—	—	—	(9.1 ± 2.0) × 10 ⁻³
1 D.B.E.									
1-Butene, 3-methyl-	C ₆ H ₁₀	149.958	0.906	0.032 ± 0.006	0.037 ± 0.007	(2.5 ± 0.5) × 10 ⁻³	(1.8 ± 0.4) × 10 ⁻³	(8.7 ± 1.7) × 10 ⁻³	0.056 ± 0.011
1-Pentene	C ₆ H ₁₀	169.952	0.924	0.030 ± 0.006	0.038 ± 0.008	—	(7.6 ± 1.5) × 10 ⁻³	(8.0 ± 1.6) × 10 ⁻³	0.10 ± 0.02
2-Methyl-1-butene	C ₆ H ₁₀	174.95	0.933	—	0.041 ± 0.008	(5.5 ± 1.1) × 10 ⁻³	—	0.013 ± 0.003	0.13 ± 0.03
2-Pentene, (E)-	C ₆ H ₁₀	184.947	0.937	0.022 ± 0.004	0.053 ± 0.011	(3.2 ± 0.6) × 10 ⁻³	(4.5 ± 0.9) × 10 ⁻³	0.015 ± 0.003	0.12 ± 0.02
2-Pentene, (Z)-	C ₆ H ₁₀	194.944	0.95	0.072 ± 0.014	0.076 ± 0.015	(5.1 ± 1.0) × 10 ⁻³	(4.0 ± 0.8) × 10 ⁻³	0.018 ± 0.004	0.23 ± 0.05
Cyclopentane	C ₅ H ₁₀	244.928	0.977	—	(2.7 ± 2.2) × 10 ⁻³	—	(5.3 ± 9.4) × 10 ⁻⁴	(3.2 ± 4.6) × 10 ⁻⁴	(4.6 ± 0.9) × 10 ⁻³
1-Pentene, 4-methyl-	C ₆ H ₁₂	234.931	0.959	(4.7 ± 0.9) × 10 ⁻³	(7.5 ± 1.5) × 10 ⁻³	(4.8 ± 1.0) × 10 ⁻⁴	(4.7 ± 0.9) × 10 ⁻⁴	(2.6 ± 0.5) × 10 ⁻⁴	0.032 ± 0.006
1-Butene, 2,3-dimethyl-	C ₆ H ₁₂	249.926	0.968	0.014 ± 0.003	0.023 ± 0.005	(7.6 ± 9.3) × 10 ⁻⁴	(1.3 ± 13.9) × 10 ⁻⁴	(6.1 ± 1.2) × 10 ⁻³	0.053 ± 0.011
1-Hexene	C ₆ H ₁₂	284.915	0.994	0.12 ± 0.02	0.16 ± 0.03	(3.2 ± 1.2) × 10 ⁻³	(5.4 ± 1.8) × 10 ⁻⁴	0.024 ± 0.005	0.36 ± 0.07
2-Hexene, (E)-	C ₆ H ₁₂	309.907	1.003	(6.5 ± 1.3) × 10 ⁻³	0.012 ± 0.002	(6.9 ± 1.4) × 10 ⁻⁴	(8.7 ± 1.7) × 10 ⁻⁴	(3.4 ± 0.7) × 10 ⁻³	0.059 ± 0.012
2-Pentene, 2-methyl-, (Z)-	C ₆ H ₁₂	314.906	1.012	0.025 ± 0.005	0.033 ± 0.007	(8.9 ± 1.8) × 10 ⁻⁴	(5.6 ± 1.1) × 10 ⁻⁴	(7.4 ± 1.5) × 10 ⁻⁴	0.049 ± 0.01
2-Pentene, 3-methyl-, (Z)-	C ₆ H ₁₂	324.902	1.021	—	0.012 ± 0.006	(5.7 ± 2.8) × 10 ⁻⁴	—	(4.1 ± 2.0) × 10 ⁻³	—
2-Hexene, (Z)-	C ₆ H ₁₂	329.901	1.016	—	—	—	(6.3 ± 1.7) × 10 ⁻⁴	—	0.026 ± 0.005
2-Pentene, 3-methyl-, (E)-	C ₆ H ₁₂	344.896	1.025	(6.3 ± 3.1) × 10 ⁻³	0.013 ± 0.006	(4.7 ± 2.4) × 10 ⁻⁴	(4.4 ± 2.2) × 10 ⁻⁴	(3.6 ± 1.8) × 10 ⁻³	0.017 ± 0.008
Cyclopentane, methyl-	C ₆ H ₁₂	359.891	1.012	(2.9 ± 0.6) × 10 ⁻³	(7.8 ± 1.6) × 10 ⁻³	—	(3.0 ± 2.4) × 10 ⁻⁴	(7.0 ± 1.4) × 10 ⁻⁴	0.024 ± 0.005
2-Pentene, 4-methyl-	C ₆ H ₁₂	369.888	1.038	(8.0 ± 4.0) × 10 ⁻⁴	(1.2 ± 0.6) × 10 ⁻³	—	—	(2.6 ± 1.3) × 10 ⁻⁴	(7.1 ± 3.6) × 10 ⁻³
Cyclohexane	C ₆ H ₁₂	434.867	1.043	—	—	(1.4 ± 0.3) × 10 ⁻⁴	(1.5 ± 0.3) × 10 ⁻⁴	—	(6.3 ± 3.8) × 10 ⁻³
1-Hexene, 3-methyl-	C ₇ H ₁₄	414.874	1.008	—	(1.6 ± 0.8) × 10 ⁻³	—	—	(3.5 ± 1.7) × 10 ⁻⁴	(7.1 ± 3.6) × 10 ⁻³
1-Hexene, 5-methyl-	C ₇ H ₁₄	429.869	1.016	—	(2.2 ± 1.1) × 10 ⁻³	—	—	(3.7 ± 1.8) × 10 ⁻⁴	(6.5 ± 3.2) × 10 ⁻³
1-Pentene, 2,3-dimethyl-	C ₇ H ₁₄	434.867	1.025	—	—	—	—	(3.7 ± 1.8) × 10 ⁻⁴	—
1-butene, 2-ethyl-, 3-methyl	C ₇ H ₁₄	449.862	1.021	(3.6 ± 1.8) × 10 ⁻³	(5.6 ± 2.8) × 10 ⁻³	—	—	(2.1 ± 1.1) × 10 ⁻³	0.016 ± 0.008
2-Hexene, 5-methyl-, (E)-	C ₇ H ₁₄	484.851	1.03	—	—	—	—	—	(4.5 ± 2.3) × 10 ⁻³
1-Heptene	C ₇ H ₁₄	509.843	1.034	0.062 ± 0.012	0.069 ± 0.014	(1.3 ± 0.3) × 10 ⁻³	(2.3 ± 0.5) × 10 ⁻³	0.013 ± 0.003	0.22 ± 0.04
3-Heptene, (E)-	C ₇ H ₁₄	529.837	1.025	(5.9 ± 8.3) × 10 ⁻⁴	(1.9 ± 1.0) × 10 ⁻³	—	—	(1.4 ± 2.2) × 10 ⁻⁴	0.016 ± 0.003
(Z)-3-Methyl-2-hexene	C ₇ H ₁₄	544.832	1.038	(2.4 ± 1.2) × 10 ⁻³	(2.6 ± 1.3) × 10 ⁻³	—	—	(1.5 ± 0.8) × 10 ⁻³	—
2-Heptene, (E)-	C ₇ H ₁₄	554.829	1.038	(4.3 ± 0.9) × 10 ⁻³	0.016 ± 0.003	—	—	—	0.054 ± 0.011
3-Methyl-2-hexene (E)	C ₇ H ₁₄	564.826	1.047	(1.0 ± 0.5) × 10 ⁻³	(1.6 ± 0.8) × 10 ⁻³	—	—	(7.3 ± 3.6) × 10 ⁻⁴	(4.5 ± 2.3) × 10 ⁻³
2-Heptene, Z	C ₇ H ₁₄	574.822	1.047	(2.9 ± 0.6) × 10 ⁻³	(4.8 ± 1.0) × 10 ⁻³	—	—	(3.4 ± 1.2) × 10 ⁻⁴	0.028 ± 0.006
C ₇ H ₁₄ isomer	C ₇ H ₁₄	579.821	1.052	—	—	—	—	(3.5 ± 1.8) × 10 ⁻⁴	—
Cyclohexane, methyl-	C ₇ H ₁₄	599.814	1.052	—	(3.3 ± 1.3) × 10 ⁻³	—	—	—	0.017 ± 0.004
Cyclopentane, ethyl-	C ₇ H ₁₄	629.805	1.052	—	(4.9 ± 1.0) × 10 ⁻³	—	—	(3.6 ± 0.7) × 10 ⁻⁴	0.021 ± 0.004
C ₈ H ₁₆ isomer	C ₈ H ₁₆	634.803	1.034	—	—	—	—	—	(5.6 ± 2.8) × 10 ⁻³
3-heptene, 2-methyl-, (Z)	C ₈ H ₁₆	684.787	1.012	—	—	—	—	—	(5.1 ± 2.6) × 10 ⁻³
1-hexene, 2,5-dimethyl-	C ₈ H ₁₆	699.782	1.025	(1.2 ± 0.6) × 10 ⁻³	(1.6 ± 0.8) × 10 ⁻³	—	—	(3.1 ± 1.8) × 10 ⁻⁴	0.014 ± 0.007
3-Heptene, 2-methyl-, (E)	C ₈ H ₁₆	719.776	1.038	—	—	—	—	—	(3.9 ± 2.0) × 10 ⁻³
1-Heptene, 5-methyl-	C ₈ H ₁₆	724.774	1.043	(1.4 ± 0.7) × 10 ⁻³	—	—	—	—	—
2-Heptene, 6-methyl-, (E)	C ₈ H ₁₆	744.768	1.043	—	—	—	—	(5.0 ± 2.5) × 10 ⁻⁴	(8.1 ± 4.1) × 10 ⁻³
2-Heptene, 6-methyl-, (Z)	C ₈ H ₁₆	761.762	1.047	—	—	—	—	—	(9.8 ± 4.9) × 10 ⁻³
Cyclohexane, 1,4-dimethyl-	C ₈ H ₁₆	764.762	1.047	(1.2 ± 0.2) × 10 ⁻³	(2.5 ± 0.5) × 10 ⁻³	(1.8 ± 0.9) × 10 ⁻³	(4.6 ± 0.9) × 10 ⁻⁴	(1.8 ± 1.8) × 10 ⁻⁴	(7.9 ± 4.0) × 10 ⁻³
1-Heptene, 2-methyl-	C ₈ H ₁₆	784.755	1.052	—	—	—	—	—	—
1-Octene	C ₈ H ₁₆	799.75	1.047	0.033 ± 0.007	0.054 ± 0.011	(1.1 ± 0.3) × 10 ⁻³	(2.1 ± 0.5) × 10 ⁻³	(8.1 ± 1.6) × 10 ⁻³	0.19 ± 0.04
3-Octene, (E)-	C ₈ H ₁₆	819.744	1.043	(1.7 ± 0.8) × 10 ⁻³	(2.0 ± 1.0) × 10 ⁻³	—	—	—	0.010 ± 0.005
2-Methyl-2-heptene	C ₈ H ₁₆	824.742	1.056	(1.6 ± 0.8) × 10 ⁻³	(1.8 ± 0.9) × 10 ⁻³	—	—	(4.3 ± 2.2) × 10 ⁻⁴	0.012 ± 0.006
2-Octene, (E)-	C ₈ H ₁₆	839.738	1.052	(3.4 ± 0.7) × 10 ⁻³	(6.5 ± 1.3) × 10 ⁻³	—	—	—	0.025 ± 0.005

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
						Giant Cutgrass	Wiregrass		
Cyclohexane, 1,3-dimethyl-, trans-	C ₈ H ₁₆	844.736	1.065	—	—	—	—	—	(3.0 ± 1.5) × 10 ⁻³
2-Octene, (Z)-	C ₈ H ₁₆	864.73	1.06	(3.4 ± 0.7) × 10 ⁻³	(3.2 ± 0.6) × 10 ⁻³	—	—	(2.0 ± 0.6) × 10 ⁻⁴	0.016 ± 0.003
Cyclopentane, 1-ethyl-2-methyl-, cis-	C ₈ H ₁₆	889.722	1.069	—	—	—	—	—	(2.5 ± 1.3) × 10 ⁻³
1-Pentene, 3-ethyl-3-methyl-	C ₈ H ₁₆	914.714	1.021	—	—	—	—	—	(3.6 ± 1.8) × 10 ⁻³
Cyclopentane, propyl-	C ₈ H ₁₆	919.712	1.069	(6.6 ± 2.2) × 10 ⁻⁴	(2.2 ± 0.4) × 10 ⁻³	—	—	—	—
Cyclohexane, ethyl-	C ₈ H ₁₆	924.71	1.082	(5.9 ± 3.0) × 10 ⁻⁴	(1.4 ± 0.7) × 10 ⁻³	—	—	—	—
C ₈ H ₁₆ isomer	C ₈ H ₁₆	1034.68	1.065	—	—	—	—	—	(4.6 ± 2.3) × 10 ⁻³
Cyclohexane, 1,1,3-trimethyl-	C ₉ H ₁₈	944.704	1.047	—	—	—	—	—	0.013 ± 0.006
C ₉ H ₁₈ isomer	C ₉ H ₁₈	974.694	1.043	(1.2 ± 0.6) × 10 ⁻³	—	—	—	(1.2 ± 0.6) × 10 ⁻³	0.023 ± 0.011
C ₉ H ₁₈ isomer	C ₉ H ₁₈	1009.68	1.052	(1.1 ± 0.6) × 10 ⁻³	—	—	—	—	—
2-Heptene, 2,6-dimethyl-	C ₉ H ₁₈	1014.68	1.043	—	(2.9 ± 1.4) × 10 ⁻³	—	—	—	—
4-Nonene, E	C ₉ H ₁₈	1074.66	1.056	—	(1.9 ± 1.0) × 10 ⁻³	—	—	—	(9.6 ± 4.8) × 10 ⁻³
1-Nonene	C ₉ H ₁₈	1089.66	1.06	0.023 ± 0.005	0.035 ± 0.007	(1.1 ± 0.5) × 10 ⁻³	(9.3 ± 7.6) × 10 ⁻⁴	(6.4 ± 1.3) × 10 ⁻³	0.14 ± 0.03
cis-4-Nonene	C ₉ H ₁₈	1099.65	1.052	(1.0 ± 0.5) × 10 ⁻³	(2.5 ± 1.2) × 10 ⁻³	—	—	—	0.015 ± 0.007
2-Nonene, (E)-	C ₉ H ₁₈	1124.65	1.065	(1.7 ± 0.3) × 10 ⁻³	(3.2 ± 0.6) × 10 ⁻³	—	—	—	0.021 ± 0.004
cis-2-Nonene	C ₉ H ₁₈	1149.64	1.074	—	(2.3 ± 0.5) × 10 ⁻³	—	—	—	0.011 ± 0.002
Cyclohexane, propyl-	C ₉ H ₁₈	1204.62	1.1	(1.7 ± 1.2) × 10 ⁻³	—	—	—	—	—
Cyclopentane, butyl-	C ₉ H ₁₈	1209.62	1.078	—	(2.8 ± 0.6) × 10 ⁻³	—	—	—	—
C ₉ H ₁₈ isomer	C ₉ H ₁₈	1249.61	1.056	(9.3 ± 4.7) × 10 ⁻⁴	(1.4 ± 0.7) × 10 ⁻³	—	—	—	(8.7 ± 4.3) × 10 ⁻³
C ₉ H ₁₈ isomer	C ₉ H ₁₈	1279.6	1.074	—	—	—	—	—	(4.9 ± 2.5) × 10 ⁻³
C ₁₀ H ₂₀ isomer	C ₁₀ H ₂₀	1144.64	1.03	—	—	—	—	(3.1 ± 4.6) × 10 ⁻⁴	0.019 ± 0.01
C ₁₀ H ₂₀ isomer	C ₁₀ H ₂₀	1269.6	1.056	—	—	—	—	—	0.013 ± 0.007
C ₁₀ H ₂₀ isomer	C ₁₀ H ₂₀	1299.59	1.06	—	—	—	—	—	0.012 ± 0.006
C ₁₀ H ₂₀ isomer	C ₁₀ H ₂₀	1349.57	1.065	—	(1.6 ± 0.8) × 10 ⁻³	—	—	—	0.013 ± 0.006
1-Decene	C ₁₀ H ₂₀	1359.57	1.074	0.023 ± 0.005	0.037 ± 0.007	(2.2 ± 0.6) × 10 ⁻³	—	(7.2 ± 1.4) × 10 ⁻³	0.13 ± 0.03
C ₁₀ H ₂₀ isomer	C ₁₀ H ₂₀	1394.56	1.074	(2.4 ± 1.2) × 10 ⁻³	(3.5 ± 2.2) × 10 ⁻³	—	—	(1.6 ± 4.6) × 10 ⁻⁴	0.023 ± 0.012
C ₁₀ H ₂₀ isomer	C ₁₀ H ₂₀	1419.55	1.082	—	(2.2 ± 1.1) × 10 ⁻³	—	—	—	0.020 ± 0.01
C ₁₀ H ₂₀ isomer	C ₁₀ H ₂₀	1479.53	1.109	—	(3.2 ± 1.6) × 10 ⁻³	—	—	—	—
C ₁₀ H ₂₀ isomer	C ₁₀ H ₂₀	1484.53	1.091	—	—	—	—	—	0.010 ± 0.006
C ₁₀ H ₂₀ isomer	C ₁₀ H ₂₀	1499.53	1.06	—	—	—	—	—	(6.9 ± 3.5) × 10 ⁻³
C ₁₀ H ₂₀ isomer	C ₁₀ H ₂₀	1589.5	1.052	—	—	—	—	—	(6.4 ± 3.2) × 10 ⁻³
C ₁₁ H ₂₂ isomer	C ₁₁ H ₂₂	1429.55	1.047	—	—	—	—	(1.6 ± 0.8) × 10 ⁻³	(6.4 ± 6.1) × 10 ⁻³
C ₁₁ H ₂₂ isomer	C ₁₁ H ₂₂	1529.52	1.065	—	—	—	—	—	(7.9 ± 3.9) × 10 ⁻³
C ₁₁ H ₂₂ isomer	C ₁₁ H ₂₂	1609.49	1.074	—	(1.7 ± 0.9) × 10 ⁻³	—	—	—	(8.9 ± 4.5) × 10 ⁻³
1-Undecene	C ₁₁ H ₂₂	1614.49	1.087	0.013 ± 0.007	0.029 ± 0.014	(7.5 ± 6.3) × 10 ⁻⁴	(7.4 ± 9.4) × 10 ⁻⁴	(4.4 ± 2.2) × 10 ⁻³	0.094 ± 0.047
C ₁₁ H ₂₂ isomer	C ₁₁ H ₂₂	1629.48	1.082	—	—	—	—	—	(4.4 ± 2.2) × 10 ⁻³
C ₁₁ H ₂₂ isomer	C ₁₁ H ₂₂	1644.48	1.091	(1.8 ± 1.8) × 10 ⁻³	(4.8 ± 2.4) × 10 ⁻³	—	—	—	0.016 ± 0.008
C ₁₁ H ₂₂ isomer	C ₁₁ H ₂₂	1669.47	1.1	—	(2.2 ± 1.1) × 10 ⁻³	—	—	—	(8.1 ± 6.1) × 10 ⁻³
C ₁₁ H ₂₂ isomer	C ₁₁ H ₂₂	1739.45	1.113	—	(1.9 ± 0.9) × 10 ⁻³	—	—	—	—
C ₁₂ H ₂₄ isomer	C ₁₂ H ₂₄	1844.42	1.087	—	—	—	—	—	0.012 ± 0.007
1-Dodecene	C ₁₂ H ₂₄	1854.41	1.096	0.013 ± 0.003	0.014 ± 0.003	—	—	(4.3 ± 0.9) × 10 ⁻³	0.098 ± 0.02
C ₁₂ H ₂₄ isomer	C ₁₂ H ₂₄	1879.4	1.1	—	(3.3 ± 2.3) × 10 ⁻³	—	—	—	0.021 ± 0.01
C ₁₂ H ₂₄ isomer	C ₁₂ H ₂₄	1884.4	1.109	—	—	—	—	—	0.013 ± 0.007
C ₁₂ H ₂₄ isomer	C ₁₂ H ₂₄	1904.4	1.109	—	—	—	—	—	0.017 ± 0.008
C ₁₂ H ₂₄ isomer	C ₁₂ H ₂₄	1919.39	1.074	—	—	—	—	—	0.011 ± 0.007
C ₁₂ H ₂₄ isomer	C ₁₂ H ₂₄	1974.37	1.135	—	—	—	—	—	0.010 ± 0.007
C ₁₂ H ₂₄ isomer	C ₁₂ H ₂₄	2069.34	1.096	—	—	—	—	—	0.015 ± 0.007
1-Tridecene	C ₁₃ H ₂₆	2074.34	1.104	(6.7 ± 3.4) × 10 ⁻³	(8.9 ± 4.4) × 10 ⁻³	—	—	(2.8 ± 1.4) × 10 ⁻³	0.053 ± 0.027
C ₁₃ H ₂₆ isomer	C ₁₃ H ₂₆	2099.33	1.109	—	—	—	—	—	0.011 ± 0.007
C ₁₃ H ₂₆ isomer	C ₁₃ H ₂₆	2124.33	1.122	—	—	—	—	—	(9.6 ± 6.6) × 10 ⁻³
C ₁₃ H ₂₆ isomer	C ₁₃ H ₂₆	2209.3	1.069	—	—	—	—	(1.6 ± 0.8) × 10 ⁻³	—
C ₁₄ H ₂₈ isomer	C ₁₄ H ₂₈	2109.33	1.082	—	—	—	—	—	0.019 ± 0.01
1-Tetradecene	C ₁₄ H ₂₈	2284.28	1.118	(5.4 ± 1.6) × 10 ⁻³	—	—	—	(2.4 ± 0.5) × 10 ⁻³	0.039 ± 0.008
1-pentadecene	C ₁₅ H ₃₀	2479.21	1.126	—	—	—	—	—	0.016 ± 0.008

23287

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
						Giant Cutgrass	Wiregrass		
2-D.B.E.									
1-Butyne, 3-methyl-	C ₆ H ₆	159.955	0.999	(8.5 ± 4.2) × 10 ⁻⁴	—	—	—	(0.4 ± 3.1) × 10 ⁻⁴	—
1,4-Pentadiene	C ₆ H ₆	164.954	0.946	0.022 ± 0.011	0.060 ± 0.03	(1.0 ± 0.5) × 10 ⁻³	(1.0 ± 0.5) × 10 ⁻³	(3.6 ± 1.8) × 10 ⁻³	0.012 ± 0.006
1-Pentyne	C ₆ H ₆	194.944	1.091	—	—	—	—	(2.0 ± 1.0) × 10 ⁻⁴	—
1,3-Pentadiene, (E)	C ₆ H ₆	204.941	1.021	0.061 ± 0.03	0.073 ± 0.036	(6.4 ± 3.2) × 10 ⁻³	(5.3 ± 2.7) × 10 ⁻³	0.021 ± 0.01	0.090 ± 0.045
1,3-Pentadiene, (Z)-	C ₆ H ₆	214.938	1.038	0.035 ± 0.018	0.049 ± 0.025	(3.2 ± 1.6) × 10 ⁻³	(2.6 ± 1.3) × 10 ⁻³	0.016 ± 0.008	0.049 ± 0.025
Cyclopentene	C ₆ H ₆	234.931	1.021	0.035 ± 0.017	0.056 ± 0.028	(1.7 ± 0.8) × 10 ⁻³	(2.8 ± 1.4) × 10 ⁻³	(7.2 ± 3.6) × 10 ⁻³	0.077 ± 0.039
2-Pentyne	C ₆ H ₆	264.922	1.17	(1.8 ± 0.9) × 10 ⁻³	(2.1 ± 1.0) × 10 ⁻³	(3.1 ± 1.5) × 10 ⁻⁴	—	(8.1 ± 4.1) × 10 ⁻⁴	—
1,4-Pentadiene, 3-methyl-	C ₆ H ₁₀	224.934	0.994	(2.0 ± 1.0) × 10 ⁻³	(2.6 ± 1.3) × 10 ⁻³	—	—	(5.1 ± 2.5) × 10 ⁻⁴	—
1,4-Pentadiene, 2-methyl-	C ₆ H ₁₀	259.923	1.03	(5.3 ± 2.6) × 10 ⁻³	(7.9 ± 3.9) × 10 ⁻³	—	—	(1.6 ± 0.8) × 10 ⁻³	(6.6 ± 3.3) × 10 ⁻³
1,5-Hexadiene	C ₆ H ₁₀	269.92	1.038	0.010 ± 0.005	0.014 ± 0.007	—	—	(1.8 ± 0.9) × 10 ⁻³	0.015 ± 0.007
1,4-Hexadiene, (E)-	C ₆ H ₁₀	299.91	1.069	(5.3 ± 2.6) × 10 ⁻³	(7.9 ± 4.0) × 10 ⁻³	—	—	(9.7 ± 4.8) × 10 ⁻⁴	(7.2 ± 3.6) × 10 ⁻³
1,4-Hexadiene, (Z)-	C ₆ H ₁₀	314.906	1.082	(4.2 ± 2.1) × 10 ⁻³	(3.9 ± 2.0) × 10 ⁻³	—	—	—	—
1,3-Pentadiene, 2-methyl-, (Z)-	C ₆ H ₁₀	324.902	1.109	0.031 ± 0.015	0.055 ± 0.027	(2.5 ± 1.3) × 10 ⁻³	—	(9.6 ± 4.8) × 10 ⁻³	—
Cyclopentene, 3-methyl-	C ₆ H ₁₀	329.901	1.056	(7.7 ± 3.9) × 10 ⁻³	(6.6 ± 3.3) × 10 ⁻³	—	(1.3 ± 0.6) × 10 ⁻³	(3.1 ± 1.6) × 10 ⁻³	0.031 ± 0.016
3-Hexyne	C ₆ H ₁₀	334.899	1.1	—	—	—	—	—	(8.3 ± 4.2) × 10 ⁻³
1,3-Butadiene, 2,3-dimethyl-	C ₆ H ₁₀	349.894	1.122	(6.8 ± 3.4) × 10 ⁻³	(5.0 ± 2.5) × 10 ⁻³	(4.7 ± 2.3) × 10 ⁻⁴	—	(2.5 ± 1.2) × 10 ⁻³	(5.2 ± 2.6) × 10 ⁻³
1,3-Hexadiene, c&t	C ₆ H ₁₀	359.891	1.131	0.013 ± 0.003	0.019 ± 0.004	(7.0 ± 2.0) × 10 ⁻⁴	(1.1 ± 0.3) × 10 ⁻³	(3.4 ± 0.7) × 10 ⁻³	0.030 ± 0.006
1,3-Pentadiene, 2-methyl-, (E)-	C ₆ H ₁₀	389.882	1.153	0.012 ± 0.006	0.019 ± 0.01	(9.1 ± 4.5) × 10 ⁻⁴	(8.8 ± 4.4) × 10 ⁻⁴	(4.9 ± 2.4) × 10 ⁻⁴	0.035 ± 0.017
4-Methyl-1,3-pentadiene	C ₆ H ₁₀	399.878	1.175	0.012 ± 0.006	0.020 ± 0.01	(6.9 ± 3.4) × 10 ⁻⁴	—	(3.9 ± 2.0) × 10 ⁻³	0.039 ± 0.019
Cyclopentene, 1-methyl-	C ₆ H ₁₀	414.874	1.104	0.023 ± 0.012	0.042 ± 0.021	(1.4 ± 0.7) × 10 ⁻³	(2.2 ± 1.1) × 10 ⁻³	(8.8 ± 4.4) × 10 ⁻³	0.076 ± 0.038
1,3-Pentadiene, 3-methyl-, (Z)-	C ₆ H ₁₀	424.87	1.184	(8.6 ± 4.3) × 10 ⁻³	0.019 ± 0.01	(7.0 ± 3.5) × 10 ⁻⁴	—	(3.8 ± 1.9) × 10 ⁻³	0.014 ± 0.007
2,4-Hexadiene, (E,E)-	C ₆ H ₁₀	439.866	1.17	(4.0 ± 0.8) × 10 ⁻³	(7.0 ± 1.4) × 10 ⁻³	—	—	(1.9 ± 0.4) × 10 ⁻³	0.015 ± 0.003
2,4-Hexadiene, (E,Z)-	C ₆ H ₁₀	464.858	1.197	(6.5 ± 1.3) × 10 ⁻³	0.011 ± 0.002	—	—	(2.5 ± 0.5) × 10 ⁻³	0.021 ± 0.004
Cyclohexene	C ₆ H ₁₀	484.851	1.157	0.026 ± 0.013	0.041 ± 0.021	(1.2 ± 0.6) × 10 ⁻³	(1.4 ± 0.7) × 10 ⁻³	(3.8 ± 1.9) × 10 ⁻³	0.063 ± 0.032
C ₇ H ₁₂ isomer	C ₇ H ₁₂	394.88	1.069	—	(2.1 ± 1.0) × 10 ⁻³	—	—	—	—
C ₇ H ₁₂ isomer	C ₇ H ₁₂	449.862	1.056	(2.2 ± 1.1) × 10 ⁻³	(2.4 ± 1.2) × 10 ⁻³	—	—	(6.8 ± 3.4) × 10 ⁻⁴	(6.7 ± 3.3) × 10 ⁻³
C ₇ H ₁₂ isomer	C ₇ H ₁₂	469.856	1.113	(1.9 ± 1.0) × 10 ⁻³	—	—	—	—	—
C ₇ H ₁₂ isomer	C ₇ H ₁₂	479.853	1.113	—	—	—	—	(8.8 ± 4.4) × 10 ⁻⁴	—
1,6-Heptadiene	C ₇ H ₁₂	489.85	1.104	(9.6 ± 4.8) × 10 ⁻³	0.014 ± 0.007	—	—	(4.8 ± 2.4) × 10 ⁻⁴	(8.1 ± 4.0) × 10 ⁻

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)			
						Giant Cutgrass	Wiregrass	Rice Straw	Indonesian Peat
C ₇ H ₁₂ isomer	C ₇ H ₁₂	744.768	1.232	—	(2.6 ± 1.3) × 10 ⁻³	—	—	(9.4 ± 4.7) × 10 ⁻⁴	(6.9 ± 3.4) × 10 ⁻³
C ₇ H ₁₂ isomer	C ₇ H ₁₂	744.768	1.245	(3.3 ± 1.6) × 10 ⁻³	(3.3 ± 1.6) × 10 ⁻³	—	—	—	—
Cyclopentane, ethylidene-	C ₇ H ₁₂	754.765	1.179	—	—	—	—	(3.9 ± 1.9) × 10 ⁻⁴	(6.0 ± 3.0) × 10 ⁻³
C ₇ H ₁₂ isomer	C ₇ H ₁₂	779.757	1.232	(3.3 ± 1.6) × 10 ⁻³	(3.5 ± 1.7) × 10 ⁻³	—	—	—	(6.9 ± 3.4) × 10 ⁻³
C ₇ H ₁₂ isomer	C ₇ H ₁₂	779.757	1.236	—	(3.0 ± 1.5) × 10 ⁻³	—	—	(7.4 ± 3.7) × 10 ⁻⁴	—
C ₈ H ₁₄ isomer	C ₈ H ₁₄	689.786	1.082	—	—	—	—	—	(3.9 ± 2.0) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	754.765	1.109	—	—	—	—	—	(4.3 ± 2.1) × 10 ⁻³
1,7-Octadiene	C ₈ H ₁₄	774.758	1.131	(6.3 ± 3.2) × 10 ⁻³	0.012 ± 0.006	—	—	(8.0 ± 4.0) × 10 ⁻⁴	(9.5 ± 4.7) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	789.754	1.126	—	—	—	—	(4.2 ± 2.1) × 10 ⁻⁴	(3.4 ± 1.7) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	794.752	1.131	—	(3.6 ± 1.8) × 10 ⁻³	—	—	—	—
C ₈ H ₁₄ isomer	C ₈ H ₁₄	814.746	1.135	—	(2.0 ± 1.0) × 10 ⁻³	—	—	—	—
C ₈ H ₁₄ isomer	C ₈ H ₁₄	824.742	1.135	(1.7 ± 0.8) × 10 ⁻³	—	—	—	(7.3 ± 3.7) × 10 ⁻⁴	—
C ₈ H ₁₄ isomer	C ₈ H ₁₄	829.741	1.144	—	(3.8 ± 1.9) × 10 ⁻³	—	—	—	—
C ₈ H ₁₄ isomer	C ₈ H ₁₄	834.739	1.144	(1.5 ± 0.7) × 10 ⁻³	—	—	—	—	(3.5 ± 1.8) × 10 ⁻³
1-Ethyl-5-methylcyclopentene	C ₈ H ₁₄	849.734	1.109	(1.3 ± 0.7) × 10 ⁻³	(2.3 ± 1.1) × 10 ⁻³	—	—	(3.5 ± 1.7) × 10 ⁻⁴	(5.8 ± 2.9) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	879.725	1.135	—	(1.8 ± 0.9) × 10 ⁻³	—	—	—	—
Cyclopentene, 3-propyl-	C ₈ H ₁₄	884.723	1.131	(2.3 ± 1.2) × 10 ⁻³	(1.8 ± 0.9) × 10 ⁻³	—	—	(4.1 ± 2.1) × 10 ⁻⁴	(8.4 ± 4.2) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	894.72	1.153	(5.2 ± 2.6) × 10 ⁻³	0.023 ± 0.012	—	—	(7.7 ± 3.8) × 10 ⁻⁴	0.011 ± 0.006
C ₈ H ₁₄ isomer	C ₈ H ₁₄	904.717	1.17	(3.2 ± 1.6) × 10 ⁻³	(7.3 ± 3.7) × 10 ⁻³	—	—	(8.7 ± 4.4) × 10 ⁻⁴	0.014 ± 0.007
C ₈ H ₁₄ isomer	C ₈ H ₁₄	904.717	1.184	(3.2 ± 1.6) × 10 ⁻³	—	—	—	—	—
C ₈ H ₁₄ isomer	C ₈ H ₁₄	914.714	1.078	—	—	—	—	—	(3.4 ± 1.7) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	929.709	1.126	—	—	—	—	(2.8 ± 1.4) × 10 ⁻⁴	(5.2 ± 2.6) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	959.699	1.14	(1.3 ± 0.6) × 10 ⁻³	(2.2 ± 1.1) × 10 ⁻³	—	—	—	(6.9 ± 3.5) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	974.694	1.188	(1.4 ± 0.7) × 10 ⁻³	(2.5 ± 1.2) × 10 ⁻³	—	—	—	—
C ₈ H ₁₄ isomer	C ₈ H ₁₄	984.691	1.206	(1.9 ± 1.0) × 10 ⁻³	(2.5 ± 1.3) × 10 ⁻³	—	—	(3.4 ± 1.7) × 10 ⁻⁴	(8.5 ± 4.3) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	1004.68	1.21	(1.5 ± 0.8) × 10 ⁻³	(2.0 ± 1.0) × 10 ⁻³	—	—	—	—
C ₈ H ₁₄ isomer	C ₈ H ₁₄	1014.68	1.219	—	(1.8 ± 0.9) × 10 ⁻³	—	—	—	—
Cyclohexane, ethylidene-	C ₈ H ₁₄	1024.68	1.197	—	(2.7 ± 1.3) × 10 ⁻³	—	—	—	(7.6 ± 3.8) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	1039.67	1.219	—	—	—	—	—	(3.8 ± 1.9) × 10 ⁻³
C ₈ H ₁₄ isomer	C ₈ H ₁₄	1099.65	1.153	—	(3.5 ± 1.7) × 10 ⁻³	—	—	—	—
C ₈ H ₁₄ isomer	C ₈ H ₁₄	999.686	1.109	(3.6 ± 10.0) × 10 ⁻⁴	(2.5 ± 1.3) × 10 ⁻³	—	—	—	—
C ₈ H ₁₆ isomer	C ₈ H ₁₆	1009.68	1.122	—	(1.3 ± 0.6) × 10 ⁻³	—	—	—	—
C ₈ H ₁₆ isomer	C ₈ H ₁₆	1019.68	1.122	—	—	—	—	—	(9.5 ± 4.8) × 10 ⁻³
C ₈ H ₁₆ isomer	C ₈ H ₁₆	1054.67	1.126	(2.2 ± 1.1) × 10 ⁻³	(5.2 ± 2.6) × 10 ⁻³	—	—	(3.1 ± 2.6) × 10 ⁻⁴	—
1,8-Nonadiene	C ₉ H ₁₆	1064.67	1.144	(7.4 ± 3.7) × 10 ⁻³	0.013 ± 0.007	—	—	(7.4 ± 3.7) × 10 ⁻⁴	(8.1 ± 4.0) × 10 ⁻³
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1079.66	1.126	—	(1.7 ± 1.2) × 10 ⁻³	—	—	(5.2 ± 2.6) × 10 ⁻⁴	(4.7 ± 2.3) × 10 ⁻³
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1089.66	1.148	—	(2.5 ± 1.3) × 10 ⁻³	—	—	—	—
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1099.65	1.148	—	—	—	—	—	(4.8 ± 2.4) × 10 ⁻³
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1124.65	1.157	—	(2.6 ± 1.3) × 10 ⁻³	—	—	—	(6.4 ± 3.2) × 10 ⁻³
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1139.64	1.157	—	(1.9 ± 0.9) × 10 ⁻³	—	—	—	—
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1144.64	1.166	(1.8 ± 1.0) × 10 ⁻³	(3.3 ± 1.6) × 10 ⁻³	—	—	(4.5 ± 2.6) × 10 ⁻⁴	0.014 ± 0.007
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1164.63	1.166	—	(2.0 ± 1.0) × 10 ⁻³	—	—	—	—
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1169.63	1.175	—	(2.3 ± 1.2) × 10 ⁻³	—	—	—	(8.5 ± 4.2) × 10 ⁻³
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1189.63	1.184	—	(6.0 ± 3.0) × 10 ⁻³	—	—	(3.2 ± 2.6) × 10 ⁻⁴	(8.0 ± 4.0) × 10 ⁻³
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1239.61	1.192	—	(6.3 ± 3.1) × 10 ⁻³	—	—	—	—
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1244.61	1.153	—	—	—	—	—	(8.8 ± 4.4) × 10 ⁻³
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1254.6	1.197	—	—	—	—	—	(6.0 ± 3.0) × 10 ⁻³
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1274.6	1.197	—	—	—	—	—	(6.5 ± 3.3) × 10 ⁻³
C ₉ H ₁₆ isomer	C ₉ H ₁₆	1274.6	1.219	—	(2.5 ± 1.3) × 10 ⁻³	—	—	—	—
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1199.62	1.109	—	(2.6 ± 2.1) × 10 ⁻³	—	—	—	—

23289

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)			
						Giant Cutgrass	Wiregrass	Rice Straw	Indonesian Peat
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1239.61	1.122	(1.3 ± 0.7) × 10 ⁻³	—	—	—	—	—
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1299.59	1.14	(1.5 ± 0.8) × 10 ⁻³	(4.9 ± 2.5) × 10 ⁻³	—	—	—	—
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1304.59	1.148	(2.2 ± 1.1) × 10 ⁻³	—	—	—	—	(8.1 ± 4.1) × 10 ⁻³
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1329.58	1.144	—	(1.7 ± 2.1) × 10 ⁻³	—	—	—	0.012 ± 0.006
1,9-Decadiene	C ₁₀ H ₁₈	1339.58	1.153	(4.8 ± 2.4) × 10 ⁻³	0.012 ± 0.006	—	—	(7.5 ± 4.6) × 10 ⁻⁴	0.012 ± 0.006
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1349.57	1.153	(2.4 ± 1.8) × 10 ⁻³	(5.7 ± 2.8) × 10 ⁻³	—	—	—	(8.2 ± 4.1) × 10 ⁻³
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1359.57	1.166	(2.1 ± 1.8) × 10 ⁻³	—	—	—	—	—
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1364.57	1.166	—	(6.5 ± 3.2) × 10 ⁻³	—	—	(2.7 ± 4.6) × 10 ⁻⁴	—
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1369.57	1.153	—	—	—	—	—	(4.8 ± 2.4) × 10 ⁻³
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1374.57	1.166	(1.3 ± 0.6) × 10 ⁻³	(2.5 ± 1.2) × 10 ⁻³	—	—	—	0.014 ± 0.007
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1384.56	1.162	(3.1 ± 1.8) × 10 ⁻³	(7.9 ± 4.0) × 10 ⁻³	—	—	(2.5 ± 4.6) × 10 ⁻⁴	—
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1394.56	1.17	(2.4 ± 1.2) × 10 ⁻³	(2.7 ± 1.4) × 10 ⁻³	—	—	—	—
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1419.55	1.179	—	(2.7 ± 2.1) × 10 ⁻³	—	—	—	—
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1434.55	1.175	—	(2.3 ± 1.1) × 10 ⁻³	—	—	—	—
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1454.54	1.197	(2.2 ± 1.1) × 10 ⁻³	(3.4 ± 1.7) × 10 ⁻³	—	—	—	0.010 ± 0.006
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1459.54	1.21	(9.3 ± 4.7) × 10 ⁻³	0.016 ± 0.008	—	—	(7.4 ± 4.6) × 10 ⁻⁴	—
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1509.52	1.17	—	(2.1 ± 1.0) × 10 ⁻³	—	—	—	(5.4 ± 2.7) × 10 ⁻³
C ₁₀ H ₁₈ isomer	C ₁₀ H ₁₈	1539.51	1.21	—	—	—	—	—	(5.6 ± 2.8) × 10 ⁻³
1,10-Undecadiene	C ₁₁ H ₂₀	1599.49	1.162	(3.2 ± 1.8) × 10 ⁻³	(6.2 ± 3.1) × 10 ⁻³	—	—	(3.5 ± 4.6) × 10 ⁻⁴	0.014 ± 0.007
C ₁₁ H ₂₀ isomer	C ₁₁ H ₂₀	1624.49	1.17	—	(2.4 ± 1.2) × 10 ⁻³	—	—	—	(5.9 ± 2.9) × 10 ⁻³
C ₁₁ H ₂₀ isomer	C ₁₁ H ₂₀	1639.48	1.157	(1.5 ± 0.8) × 10 ⁻³	—	—	—	—	—
C ₁₁ H ₂₀ isomer	C ₁₁ H ₂₀	1704.46	1.206	(2.2 ± 1.8) × 10 ⁻³	(3.0 ± 1.5) × 10 ⁻³	—	—	—	(7.1 ± 3.6) × 10 ⁻³
C ₁₁ H ₂₀ isomer	C ₁₁ H ₂₀	1719.46	1.197	—	(2.5 ± 1.2) × 10 ⁻³	—	—	—	—
C ₁₂ H ₂₂ isomer	C ₁₂ H ₂₂	1719.46	1.192	(2.9 ± 1.9) × 10 ⁻³	—	—	—	—	—
1,11-Dodecadiene	C ₁₂ H ₂₂	1834.42	1.17	(8.5 ± 4.3) × 10 ⁻³	0.010 ± 0.005	—	—	—	0.014 ± 0.007
1,12-Tridecadiene	C ₁₃ H ₂₄	2059.35	1.175	(2.9 ± 1.9) × 10 ⁻³	(3.5 ± 2.3) × 10 ⁻³	—	—	—	0.013 ± 0.007
C ₁₄ H ₂₆ isomer	C ₁₄ H ₂₆	2234.29	1.285	—	—	—	—	—	0.022 ± 0.011
3 D.B.E.									
1-Buten-3-yne, 2-methyl-	C ₆ H ₈	174.95	1.144	(2.2 ± 1.2) × 10 ⁻³	(2.4 ± 1.4) × 10 ⁻³	—	—	(2.0 ± 3.1) × 10 ⁻⁴	—
4-Penten-1-yne	C ₆ H ₈	209.939	1.307	(9.2 ± 12.0) × 10 ⁻⁴	(3.7 ± 1.8) × 10 ⁻³	(3.0 ± 1.5) × 10 ⁻⁴	—	—	(3.6 ± 3.1) × 10 ⁻⁴
1,3-Cyclopentadiene	C ₅ H ₆	219.936	1.126	0.14 ± 0.07	0.18 ± 0.09	0.032 ± 0.016	(9.4 ± 4.7) × 10 ⁻³	0.036 ± 0.018	0.063 ± 0.032
3-Penten-1-yne, (E)-	C ₆ H ₈	224.934	1.417	(1.4 ± 0.7) × 10 ⁻³	(3.4 ± 1.7) × 10 ⁻³	(6.0 ± 3.0) × 10 ⁻⁴	—	—	(1.4 ± 3.1) × 10 ⁻⁴
1-Penten-3-yne	C ₆ H ₈	229.933	1.153	(3.3 ± 1.6) × 10 ⁻³	—	—	—	—	(9.1 ± 4.6) × 10 ⁻⁴
3-Penten-1-yne, (Z)-	C ₆ H ₈	269.92	1.373	(7.4 ± 3.7) × 10 ⁻³	(6.5 ± 3.3) × 10 ⁻³	(1.4 ± 0.7) × 10 ⁻³	—	—	(2.9 ± 1.4) × 10 ⁻³
1-Hexen-3-yne	C ₆ H ₈	309.907	1.219	(2.7 ± 1.3) × 10 ⁻³	(6.3 ± 3.2) × 10 ⁻³	—	—	—	(8.1 ± 4.0) × 10 ⁻⁴
2-Hexene-4-yne	C ₆ H ₈	529.837	1.514	—	—	—	—	—	(3.3 ± 2.5) × 10 ⁻⁴
1,3-Cyclopentadiene, 1-methyl-	C ₆ H ₈	394.88	1.267	0.061 ± 0.031	0.091 ± 0.045	(5.0 ± 2.5) × 10 ⁻³	(3.6 ± 1.8) × 10 ⁻³	0.013 ± 0.007	0.047 ± 0.023
1,3-Cyclopentadiene, 1-methyl-	C ₆ H ₈	404.877	1.289	0.054 ± 0.027	0.078 ± 0.039	(4.2 ± 2.1) × 10 ⁻³	(2.9 ± 1.5) × 10 ⁻³	0.011 ± 0.006	0.039 ± 0.02
1,3-Cyclohexadiene	C ₆ H ₈	464.858	1.316	—	0.069 ± 0.014	(2.0 ± 0.4) × 10 ⁻³	(2.2 ± 0.5) × 10 ⁻³	(6.7 ± 1.3) × 10 ⁻³	—
1,4-Cyclohexadiene	C ₆ H ₈	559.827	1.39	—	(1.6 ± 0.4) × 10 ⁻³	—	—	—	—
C ₇ H ₁₀ isomer	C ₇ H ₁₀	549.83	1.232	(3.6 ± 1.8) × 10 ⁻³	—	—	—	—	—
C ₇ H ₁₀ isomer	C ₇ H ₁₀	554.829	1.21	—	(2.7 ± 1.3) × 10 ⁻³	—	—	—	—
C ₇ H ₁₀ isomer	C ₇ H ₁₀	589.818	1.25	(1.0 ± 0.9) × 10 ⁻³	(1.2 ± 1.1) × 10 ⁻³	—	—	—	—
C ₇ H ₁₀ isomer	C ₇ H ₁₀	604.813	1.267	—	(2.2 ± 1.1) × 10 ⁻³	—	—	(1.4 ± 2.5) × 10 ⁻⁴	—
C ₇ H ₁₀ isomer	C ₇ H ₁₀	619.808	1.28	—	—	—	—	—	(4.4 ± 2.2) × 10 ⁻³
C ₇ H ₁₀ isomer	C ₇ H ₁₀	624.806	1.276	(3.5 ± 1.7) × 10 ⁻³	(5.4 ± 2.7) × 10 ⁻³	—	—	(4.2 ± 2.5) × 10 ⁻⁴	—
C ₇ H ₁₀ isomer	C ₇ H ₁₀	669.792	1.302	0.012 ± 0.006	0.019 ± 0.01	—	(9.2 ± 5.0) × 10 ⁻⁴	(9.9 ± 4.9) × 10 ⁻⁴	0.020 ± 0.01
C ₇ H ₁₀ isomer	C ₇ H ₁₀	679.789	1.316	(4.8 ± 2.4) × 10 ⁻³	(3.0 ± 1.5) × 10 ⁻³	—	—	—	(5.1 ± 3.3) × 10 ⁻³
C ₇ H ₁₀ isomer	C ₇ H ₁₀	679.789	1.324	—	(5.0 ± 2.5) × 10 ⁻³	—	—	(5.3 ± 2.7) × 10 ⁻⁴	—

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)			
						Giant Cutgrass	Wiregrass	Rice Straw	Indonesian Peat
C ₇ H ₁₀ isomer	C ₇ H ₁₀	689.786	1.32	0.031 ± 0.016	0.013 ± 0.006	–	(2.8 ± 5.0) × 10 ⁻⁴	(6.0 ± 3.0) × 10 ⁻⁴	0.013 ± 0.007
C ₇ H ₁₀ isomer	C ₇ H ₁₀	714.778	1.342	0.026 ± 0.013	0.022 ± 0.011	–	(2.7 ± 5.0) × 10 ⁻⁴	(7.0 ± 3.5) × 10 ⁻⁴	0.015 ± 0.007
C ₇ H ₁₀ isomer	C ₇ H ₁₀	734.771	1.346	–	0.018 ± 0.009	–	–	(2.4 ± 2.5) × 10 ⁻⁴	(7.4 ± 3.7) × 10 ⁻³
C ₇ H ₁₀ isomer	C ₇ H ₁₀	754.765	1.355	(5.7 ± 2.9) × 10 ⁻³	(6.1 ± 3.1) × 10 ⁻³	–	–	(7.2 ± 3.6) × 10 ⁻⁴	–
C ₇ H ₁₀ isomer	C ₇ H ₁₀	764.762	1.36	(1.8 ± 0.9) × 10 ⁻³	(5.9 ± 2.9) × 10 ⁻³	–	–	–	–
C ₇ H ₁₀ isomer	C ₇ H ₁₀	774.758	1.364	(7.3 ± 3.7) × 10 ⁻³	–	–	–	(1.3 ± 0.6) × 10 ⁻³	(7.8 ± 3.9) × 10 ⁻³
C ₇ H ₁₀ isomer	C ₇ H ₁₀	769.76	1.386	–	0.015 ± 0.007	–	–	–	–
C ₇ H ₁₀ isomer	C ₇ H ₁₀	834.739	1.404	(2.6 ± 1.3) × 10 ⁻³	(5.2 ± 2.6) × 10 ⁻³	–	–	–	(4.4 ± 2.2) × 10 ⁻³
C ₈ H ₁₂ isomer	C ₈ H ₁₂	874.726	1.276	(2.1 ± 1.0) × 10 ⁻³	(5.8 ± 2.9) × 10 ⁻³	–	–	–	(3.7 ± 1.9) × 10 ⁻³
C ₈ H ₁₂ isomer	C ₈ H ₁₂	889.722	1.28	(1.6 ± 0.8) × 10 ⁻³	(1.3 ± 0.7) × 10 ⁻³	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	919.712	1.298	–	(1.4 ± 0.7) × 10 ⁻³	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	924.71	1.311	–	(2.2 ± 1.1) × 10 ⁻³	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	929.709	1.302	(1.2 ± 0.9) × 10 ⁻³	–	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	939.706	1.324	(9.6 ± 4.8) × 10 ⁻⁴	(3.9 ± 1.9) × 10 ⁻³	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	959.699	1.32	–	(2.3 ± 1.1) × 10 ⁻³	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	979.693	1.311	(3.6 ± 1.8) × 10 ⁻³	(1.3 ± 1.1) × 10 ⁻³	–	–	–	(3.0 ± 3.2) × 10 ⁻³
C ₈ H ₁₂ isomer	C ₈ H ₁₂	979.693	1.324	–	(1.5 ± 1.1) × 10 ⁻³	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	989.69	1.263	(1.4 ± 0.7) × 10 ⁻³	(1.8 ± 0.9) × 10 ⁻³	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	994.688	1.338	(1.3 ± 0.7) × 10 ⁻³	(6.1 ± 3.1) × 10 ⁻³	–	–	–	(4.3 ± 2.2) × 10 ⁻³
C ₈ H ₁₂ isomer	C ₈ H ₁₂	1009.68	1.351	–	(1.3 ± 1.1) × 10 ⁻³	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	1024.68	1.36	(1.3 ± 0.6) × 10 ⁻³	(2.9 ± 1.4) × 10 ⁻³	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	1034.68	1.355	(5.6 ± 2.8) × 10 ⁻³	(2.9 ± 1.4) × 10 ⁻³	–	–	–	(4.3 ± 2.1) × 10 ⁻³
C ₈ H ₁₂ isomer	C ₈ H ₁₂	1059.67	1.404	(2.5 ± 1.2) × 10 ⁻³	0.010 ± 0.005	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	1079.66	1.395	–	(4.2 ± 2.1) × 10 ⁻³	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	1089.66	1.377	(3.3 ± 1.6) × 10 ⁻³	(3.1 ± 1.6) × 10 ⁻³	–	–	–	(3.9 ± 2.0) × 10 ⁻³
C ₈ H ₁₂ isomer	C ₈ H ₁₂	1109.65	1.412	(1.6 ± 0.9) × 10 ⁻³	–	–	–	–	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	1139.64	1.399	–	(2.4 ± 1.2) × 10 ⁻³	–	–	–	(3.9 ± 1.9) × 10 ⁻³
C ₈ H ₁₂ isomer	C ₈ H ₁₂	1144.64	1.452	–	(2.5 ± 1.3) × 10 ⁻³	–	–	–	–
C ₉ H ₁₄ isomer	C ₉ H ₁₄	939.706	1.192	(9.6 ± 4.8) × 10 ⁻⁴	(1.5 ± 0.8) × 10 ⁻³	–	–	–	(9.7 ± 4.9) × 10 ⁻³
C ₉ H ₁₄ isomer	C ₉ H ₁₄	954.701	1.188	–	–	–	–	–	(6.6 ± 3.3) × 10 ⁻³
C ₉ H ₁₄ isomer	C ₉ H ₁₄	1029.68	1.258	–	–	–	–	–	(3.2 ± 1.6) × 10 ⁻³
C ₉ H ₁₄ isomer	C ₉ H ₁₄	1069.66	1.113	–	–	–	–	–	(9.6 ± 4.8) × 10 ⁻³
C ₉ H ₁₄ isomer	C ₉ H ₁₄	1089.66	1.228	(9.3 ± 10.0) × 10 ⁻⁴	(6.7 ± 12.1) × 10 ⁻⁴	–	–	(2.8 ± 2.6) × 10 ⁻⁴	–
C ₉ H ₁₄ isomer	C ₉ H ₁₄	1099.65	1.254	–	(8.1 ± 12.1) × 10 ⁻⁴	–	–	–	–
C ₉ H ₁₄ isomer	C ₉ H ₁₄	1124.65	1.245	0.010 ± 0.005	(3.2 ± 1.6) × 10 ⁻³	–	–	–	–
C ₉ H ₁₄ isomer	C ₉ H ₁₄	1154.64	1.236	–	(2.0 ± 1.2) × 10 ⁻³	–	–	–	–
C ₉ H ₁₄ isomer	C ₉ H ₁₄	1194.62	1.302	–	(1.3 ± 1.2) × 10 ⁻³	–	–	–	–
C ₉ H ₁₄ isomer	C ₉ H ₁₄	1214.62	1.298	–	(2.3 ± 1.2) × 10 ⁻³	–	–	–	–
C ₉ H ₁₄ isomer	C ₉ H ₁₄	1229.61	1.32	–	(6.7 ± 12.1) × 10 ⁻⁴	–	–	–	–
C ₉ H ₁₄ isomer	C ₉ H ₁₄	1259.6	1.355	–	(2.3 ± 1.2) × 10 ⁻³	–	–	–	–
C ₁₁ H ₁₈	C ₁₁ H ₁₈	1794.43	1.342	(2.9 ± 1.9) × 10 ⁻³	(3.9 ± 2.3) × 10 ⁻³	–	–	–	–
Other									
1,5-Hexadien-3-yne	C ₈ H ₈	404.877	1.659	(7.8 ± 3.9) × 10 ⁻³	(8.9 ± 4.5) × 10 ⁻³	(5.1 ± 8.7) × 10 ⁻⁴	(5.5 ± 2.7) × 10 ⁻⁴	(2.3 ± 1.2) × 10 ⁻³	(3.2 ± 1.6) × 10 ⁻³
1,5-Hexadiyne	C ₈ H ₈	439.866	1.69	(4.9 ± 2.5) × 10 ⁻⁴	(8.6 ± 4.3) × 10 ⁻⁴	–	–	–	–
C ₇ H ₈ isomer	C ₇ H ₈	679.789	1.632	(3.5 ± 1.8) × 10 ⁻³	(2.6 ± 1.3) × 10 ⁻³	–	–	(8.7 ± 4.3) × 10 ⁻⁴	(2.1 ± 1.1) × 10 ⁻³
C ₇ H ₈ isomer	C ₇ H ₈	714.778	1.672	(4.4 ± 2.2) × 10 ⁻³	(2.0 ± 1.0) × 10 ⁻³	–	–	(5.1 ± 2.6) × 10 ⁻⁴	–
C ₇ H ₈ isomer	C ₇ H ₈	859.731	1.936	–	(1.1 ± 0.5) × 10 ⁻³	–	–	–	–
1,3,5-Cycloheptatriene	C ₇ H ₈	864.73	1.918	(1.1 ± 0.5) × 10 ⁻³	–	–	(2.3 ± 1.2) × 10 ⁻⁴	(7.5 ± 3.8) × 10 ⁻⁴	–
C ₈ H ₈ isomer	C ₈ H ₈	1219.62	1.888	(1.9 ± 0.9) × 10 ⁻³	(1.6 ± 0.8) × 10 ⁻³	(3.9 ± 4.0) × 10 ⁻⁴	–	(2.3 ± 2.9) × 10 ⁻⁴	–
C ₈ H ₁₀ isomer	C ₈ H ₁₀	1039.67	1.641	(2.3 ± 1.1) × 10 ⁻³	–	–	–	–	–

23291

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)			
						Giant Cutgrass	Wiregrass	Rice Straw	Indonesian Peat
C ₈ H ₁₀ isomer	C ₈ H ₁₀	1044.67	1.602	–	(1.7 ± 0.9) × 10 ⁻³	–	–	–	–
C ₈ H ₁₀ isomer	C ₈ H ₁₀	1074.66	1.65	(1.2 ± 0.6) × 10 ⁻³	(1.9 ± 1.0) × 10 ⁻³	–	–	–	–
C ₈ H ₁₀ isomer	C ₈ H ₁₀	1144.64	1.786	–	(1.8 ± 0.9) × 10 ⁻³	–	–	–	–
C ₈ H ₁₀ isomer	C ₈ H ₁₀	1154.64	1.76	–	–	–	–	(5.6 ± 2.8) × 10 ⁻⁴	–
C ₈ H ₁₂ isomer	C ₈ H ₁₂	1014.68	1.267	(2.4 ± 1.2) × 10 ⁻³	–	–	–	–	–
C ₁₀ H ₁₄ isomer	C ₁₀ H ₁₄	1169.63	1.267	(5.1 ± 2.5) × 10 ⁻³	–	–	–	–	–
C ₁₀ H ₁₄ isomer	C ₁₀ H ₁₄	1304.59	1.28	(1.3 ± 0.6) × 10 ⁻³	–	–	–	–	–
C ₁₀ H ₁₄ isomer	C ₁₀ H ₁₄	1334.58	1.412	(1.9 ± 0.9) × 10 ⁻³	(4.4 ± 2.2) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₄ isomer	C ₁₀ H ₁₄	1404.56	1.443	–	(6.6 ± 3.3) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₄ isomer	C ₁₀ H ₁₄	1409.56	1.434	(2.1 ± 1.0) × 10 ⁻³	–	–	–	–	–
C ₁₀ H ₁₄ isomer	C ₁₀ H ₁₄	1464.54	1.487	–	(7.3 ± 3.6) × 10 ⁻³	–	–	–	–
C ₁₁ H ₁₆ isomer	C ₁₁ H ₁₆	1629.48	1.465	–	(1.6 ± 0.8) × 10 ⁻³	–	–	–	–
Terpenoids									
Other									
Isoprene	C ₅ H ₈	189.946	0.994	0.28 ± 0.06	0.40 ± 0.08	0.030 ± 0.006	0.012 ± 0.002	0.088 ± 0.018	0.31 ± 0.06
Santene	C ₉ H ₁₄	1069.66	1.157	0.12 ± 0.06	–	–	–	–	–
Bornyl Acetate	C ₁₂ H ₂₀ O ₂	2094.34	1.628	0.040 ± 0.02	–	–	–	–	–
Monoterpenes									
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1069.66	1.091	–	(1.2 ± 0.6) × 10 ⁻³	–	–	–	–
Bornylene	C ₁₀ H ₁₆	1129.64	1.144	(8.7 ± 4.3) × 10 ⁻³	–	–	–	–	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1159.64	1.228	–	(2.2 ± 1.1) × 10 ⁻³	–	–	–	–
gamma pyronene	C ₁₀ H ₁₆	1174.63	1.197	0.017 ± 0.008	(8.8 ± 4.4) × 10 ⁻³	–	–	(5.0 ± 2.5) × 10 ⁻⁴	–
Tricyclene	C ₁₀ H ₁₆	1189.63	1.153	0.20 ± 0.1	–	–	–	–	–
a-thujene	C ₁₀ H ₁₆	1194.62	1.157	–	(8.9 ± 4.5) × 10 ⁻³	–	–	–	–
α-Pinene	C ₁₀ H ₁₆	1219.62	1.157	0.17 ± 0.03	0.082 ± 0.016	–	–	(8.6 ± 7.3) × 10 ⁻⁴	–
C10H16 isomer	C ₁₀ H ₁₆	1244.61	1.192	(6.3 ± 3.2) × 10 ⁻³	(3.1 ± 1.6) × 10 ⁻³	–	–	–	–
α-Fenchene	C ₁₀ H ₁₆	1254.6	1.201	(5.0 ± 2.5) × 10 ⁻³	(8.8 ± 4.4) × 10 ⁻³	–	–	–	–
Camphene	C ₁₀ H ₁₆	1264.6	1.228	0.44 ± 0.09	0.017 ± 0.003	–	–	–	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1279.6	1.232	0.018 ± 0.009	0.011 ± 0.006	–	–	–	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1284.6	1.232	(9.3 ± 2.2) × 10 ⁻³	–	–	–	–	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1289.59	1.245	(9.9 ± 4.9) × 10 ⁻³	0.017 ± 0.008	–	–	(2.1 ± 1.0) × 10 ⁻³	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1299.59	1.236	(1.5 ± 0.8) × 10 ⁻³	(5.4 ± 2.7) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1309.59	1.223	(3.7 ± 1.9) × 10 ⁻³	(1.5 ± 0.8) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1319.58	1.245	–	(1.6 ± 0.8) × 10 ⁻³	–	–	–	–
Sabinene	C ₁₀ H ₁₆	1329.58	1.267	0.022 ± 0.004	(5.2 ± 1.3) × 10 ⁻³	–	–	–	–
b-Pinene	C ₁₀ H ₁₆	1339.58	1.254	0.089 ± 0.018	0.23 ± 0.05	–	–	–	–
b-pyronene	C ₁₀ H ₁₆	1354.57	1.28	0.018 ± 0.009	–	–	–	–	–
b-Myrcene	C ₁₀ H ₁₆	1364.57	1.28	0.13 ± 0.03	0.22 ± 0.04	–	–	–	(6.8 ± 3.9) × 10 ⁻³
pyronene?	C ₁₀ H ₁₆	1384.56	1.276	–	(2.7 ± 1.3) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1394.56	1.245	(4.0 ± 2.0) × 10 ⁻³	(4.9 ± 2.4) × 10 ⁻³	–	–	–	–
α-Phellandrene	C ₁₀ H ₁₆	1414.55	1.302	0.013 ± 0.003	0.016 ± 0.003	–	–	–	–
3-Carene	C ₁₀ H ₁₆	1424.55	1.267	0.14 ± 0.03	0.18 ± 0.04	–	–	–	–
Alpha terpinene	C ₁₀ H ₁₆	1444.54	1.311	0.016 ± 0.003	0.011 ± 0.002	–	–	–	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1459.54	1.307	(1.8 ± 0.9) × 10 ⁻³	–	–	–	–	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1464.54	1.316	(2.3 ± 1.2) × 10 ⁻³	–	–	–	–	–
Limonene	C ₁₀ H ₁₆	1474.53	1.329	0.23 ± 0.05	0.17 ± 0.03	(1.3 ± 1.0) × 10 ⁻³	(2.0 ± 1.5) × 10 ⁻³	0.018 ± 0.004	–
2-Ocimene	C ₁₀ H ₁₆	1479.53	1.338	–	0.038 ± 0.008	–	–	–	–
b-Phellandrene	C ₁₀ H ₁₆	1484.53	1.36	0.047 ± 0.023	0.024 ± 0.012	–	–	(8.8 ± 4.4) × 10 ⁻⁴	–
C ₁₀ H ₁₆ isomer	C ₁₀ H ₁₆	1499.53	1.32	(2.7 ± 1.3) × 10 ⁻³	(5.1 ± 2.6) × 10 ⁻³	–	–	–	–

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
						Giant Cutgrass	Wiregrass		
(E)-Ocimene									
C ₁₀ H ₁₆		1514.52	1.355	(4.4 ± 0.9) × 10 ⁻³	(5.4 ± 1.1) × 10 ⁻³	–	–	–	–
Gamma terpinene									
C ₁₀ H ₁₆		1544.51	1.364	(6.0 ± 1.4) × 10 ⁻³	(7.7 ± 1.8) × 10 ⁻³	–	–	–	–
C ₁₀ H ₁₆ isomer		1589.5	1.382	(2.7 ± 1.4) × 10 ⁻³	(6.1 ± 3.0) × 10 ⁻³	–	–	–	–
Terpinolene									
C ₁₀ H ₁₆		1619.49	1.39	0.038 ± 0.008	0.035 ± 0.007	–	–	–	–
Allo-ocimene or α-pyrone									
C ₁₀ H ₁₆		1729.45	1.443	(4.7 ± 2.4) × 10 ⁻³	(6.4 ± 3.2) × 10 ⁻³	–	–	–	–
1,3-Cyclohexadiene, 5-butyl-		1754.44	1.333	(1.3 ± 0.6) × 10 ⁻³	–	–	–	–	–
Allo-ocimene or α-pyrone		1764.44	1.474	(1.8 ± 0.9) × 10 ⁻³	(2.4 ± 1.2) × 10 ⁻³	–	–	–	–
Sesquiterpenes (and related)									
α-Calacorene	C ₁₅ H ₂₀	2624.17	1.822	–	–	–	–	–	0.013 ± 0.006
Calamenene	C ₁₅ H ₂₂	2579.18	1.654	(6.8 ± 3.4) × 10 ⁻³	–	–	–	–	0.018 ± 0.009
α-Cubebene	C ₁₅ H ₂₄	2229.29	1.241	(5.1 ± 2.5) × 10 ⁻³	–	–	–	–	–
Copaene	C ₁₅ H ₂₄	2294.27	1.28	(4.9 ± 2.4) × 10 ⁻³	(4.9 ± 2.4) × 10 ⁻³	–	–	–	–
C ₁₅ H ₂₄ isomer	C ₁₅ H ₂₄	2319.26	1.39	(8.4 ± 4.2) × 10 ⁻³	0.012 ± 0.006	–	–	–	–
Germacrene D	C ₁₅ H ₂₄	2379.24	1.36	(6.1 ± 3.0) × 10 ⁻³	–	–	–	–	–
B-Caryophyllene									
C ₁₅ H ₂₄		2394.24	1.404	(7.3 ± 1.5) × 10 ⁻³	–	–	–	–	–
C ₁₅ H ₂₄ isomer	C ₁₅ H ₂₄	2404.24	1.373	(5.6 ± 2.8) × 10 ⁻³	–	–	–	–	–
C ₁₅ H ₂₄ isomer	C ₁₅ H ₂₄	2454.22	1.47	–	(7.3 ± 3.7) × 10 ⁻³	–	–	–	–
Cadinene isomer	C ₁₅ H ₂₄	2484.21	1.448	(9.6 ± 4.8) × 10 ⁻³	(7.5 ± 3.7) × 10 ⁻³	–	–	–	–
Cadinene isomer	C ₁₅ H ₂₄	2529.2	1.456	(9.9 ± 5.0) × 10 ⁻³	(5.5 ± 2.8) × 10 ⁻³	–	–	–	–
Cadinene isomer	C ₁₅ H ₂₄	2564.19	1.492	0.028 ± 0.014	(8.4 ± 4.2) × 10 ⁻³	–	–	–	–
Cadinene isomer	C ₁₅ H ₂₄	2604.17	1.536	(5.0 ± 2.5) × 10 ⁻³	–	–	–	–	–
Ledane	C ₁₅ H ₂₆	2414.23	1.355	–	–	–	–	–	0.019 ± 0.009
C ₁₅ H ₂₆ isomer	C ₁₅ H ₂₆	2504.2	1.373	–	–	–	–	–	0.017 ± 0.009
Patchulane	C ₁₅ H ₂₆	2549.19	1.448	–	–	–	–	–	0.023 ± 0.012
Oxygenated Aliphatic Compounds									
Aldehydes									
Acrolein									
C ₂ H ₂ O		169.952	1.426	0.22 ± 0.04	0.26 ± 0.05	0.035 ± 0.007	0.027 ± 0.005	0.062 ± 0.012	0.057 ± 0.019
Propanal	C ₃ H ₄ O	174.95	1.241	(9.5 ± 5.1) × 10 ⁻³	0.010 ± 0.01	(6.8 ± 3.4) × 10 ⁻³	–	0.013 ± 0.006	0.039 ± 0.025
Methacrolein									
C ₄ H ₆ O		259.923	1.571	0.073 ± 0.015	0.10 ± 0.02	(8.4 ± 4.2) × 10 ⁻³	(7.7 ± 1.5) × 10 ⁻³	0.023 ± 0.005	0.061 ± 0.012
2-Butenal	C ₄ H ₆ O	419.872	2.517	0.079 ± 0.04	0.15 ± 0.07	(8.4 ± 4.2) × 10 ⁻³	0.022 ± 0.011	0.042 ± 0.021	0.017 ± 0.013
Propanal, 2-methyl-	C ₄ H ₈ O	239.93	1.298	0.020 ± 0.01	0.043 ± 0.021	(1.2 ± 1.3) × 10 ⁻³	–	0.013 ± 0.007	0.15 ± 0.07
Acetaldehyde, methoxy-									
Butanal	C ₄ H ₈ O	279.917	2.592	–	(2.5 ± 1.2) × 10 ⁻³	–	–	–	–
C ₄ H ₈ O		289.914	1.558	0.015 ± 0.004	0.031 ± 0.006	–	(3.6 ± 2.0) × 10 ⁻³	0.016 ± 0.003	(6.7 ± 12.9) × 10 ⁻³
Pent-2-ynal	C ₅ H ₈ O	484.851	2.512	(1.3 ± 0.6) × 10 ⁻³	(1.8 ± 0.9) × 10 ⁻³	–	–	–	–
2-Ethylacrolein	C ₅ H ₈ O	464.858	1.756	(3.7 ± 1.8) × 10 ⁻³	(4.4 ± 2.2) × 10 ⁻³	–	–	(2.6 ± 1.3) × 10 ⁻³	–
4-Pentenal	C ₅ H ₈ O	499.846	2.182	(1.7 ± 0.8) × 10 ⁻³	(3.4 ± 1.7) × 10 ⁻³	–	–	(8.1 ± 4.0) × 10 ⁻⁴	–
2-Butenal, 2-methyl-	C ₅ H ₈ O	669.792	2.174	(3.9 ± 1.9) × 10 ⁻³	(8.5 ± 4.2) × 10 ⁻³	–	–	(2.5 ± 1.2) × 10 ⁻³	(6.3 ± 3.2) × 10 ⁻³
2-Pentenal, (E)-	C ₅ H ₈ O	704.781	2.345	–	(2.9 ± 1.4) × 10 ⁻³	–	–	–	–
2-Butenal, 3-methyl-	C ₅ H ₈ O	794.752	2.658	(1.8 ± 0.9) × 10 ⁻³	(3.6 ± 1.8) × 10 ⁻³	–	–	(8.8 ± 4.4) × 10 ⁻⁴	–
2-pentenal	C ₅ H ₈ O	794.752	2.662	–	–	–	–	(4.3 ± 2.2) × 10 ⁻³	–
Butanal, 3-methyl-	C ₆ H ₁₀ O	429.869	1.558	0.017 ± 0.009	0.046 ± 0.023	(8.3 ± 4.2) × 10 ⁻⁴	(2.5 ± 1.2) × 10 ⁻³	(8.1 ± 4.0) × 10 ⁻³	0.11 ± 0.06
Butanal, 2-methyl-	C ₆ H ₁₀ O	449.862	1.514	(5.4 ± 2.7) × 10 ⁻³	0.022 ± 0.011	(5.7 ± 2.8) × 10 ⁻⁴	(1.2 ± 0.6) × 10 ⁻³	(5.0 ± 2.5) × 10 ⁻³	0.071 ± 0.035
Pentanal	C ₆ H ₁₀ O	529.837	1.707	0.016 ± 0.003	0.020 ± 0.004	–	(1.1 ± 0.6) × 10 ⁻³	–	0.014 ± 0.005
Hexanal	C ₆ H ₁₂ O	829.741	1.694	(9.9 ± 2.5) × 10 ⁻³	0.011 ± 0.003	–	–	(1.5 ± 0.7) × 10 ⁻³	0.011 ± 0.007
Heptanal	C ₇ H ₁₄ O	1124.65	1.663	(7.0 ± 3.5) × 10 ⁻³	(8.7 ± 4.3) × 10 ⁻³	–	–	–	0.017 ± 0.009
Octanal	C ₈ H ₁₆ O	1399.56	1.632	(2.6 ± 1.4) × 10 ⁻³	–	–	–	–	–
Nonanal	C ₉ H ₁₈ O	1659.48	1.606	(3.9 ± 1.9) × 10 ⁻³	–	–	(2.9 ± 1.4) × 10 ⁻³	–	–
Decanal	C ₁₀ H ₂₀ O	1899.4	1.584	–	–	(1.6 ± 0.3) × 10 ⁻³	–	–	–

23293

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
						Giant Cutgrass	Wiregrass		
Dodecanal	C ₁₂ H ₂₄ O	2329.26	1.566	–	–	(2.0 ± 1.0) × 10 ⁻³	–	–	(4.8 ± 3.1) × 10 ⁻³
Ketones									
Acetone									
C ₃ H ₆ O	174.95	1.32	0.13 ± 0.03	0.25 ± 0.05	–	–	0.036 ± 0.007	0.11 ± 0.02	0.37 ± 0.07
Hydroxyacetone	C ₃ H ₆ O ₂	444.864	3.846	(9.0 ± 4.5) × 10 ⁻³	0.052 ± 0.026	0.010 ± 0.005	(9.7 ± 4.9) × 10 ⁻³	0.11 ± 0.06	–
Methyl vinyl ketone									
C ₄ H ₆ O	289.914	2.015	0.19 ± 0.04	0.29 ± 0.06	0.028 ± 0.006	0.038 ± 0.008	0.13 ± 0.03	0.093 ± 0.019	–
2,3-Butanedione	C ₄ H ₆ O ₂	289.914	2.253	0.098 ± 0.049	0.18 ± 0.09	(7.6 ± 3.8) × 10 ⁻³	0.049 ± 0.025	0.056 ± 0.028	0.043 ± 0.022
2-Butanone									
C ₄ H ₈ O	299.91	1.685	0.038 ± 0.008	0.12 ± 0.02	(4.9 ± 1.0) × 10 ⁻³	0.016 ± 0.003	0.068 ± 0.014	0.10 ± 0.02	–
2-Butanone, 3-hydroxy-	C ₄ H ₈ O ₂	564.826	1.065	–	–	–	–	(5.0 ± 2.5) × 10 ⁻³	–
1-Hydroxy-2-butanone	C ₄ H ₈ O ₂	724.774	1.514	–	–	–	–	(6.5 ± 3.3) × 10 ⁻³	–
3-Cyclopentene-1,2-dione	C ₅ H ₄ O ₂	1054.67	0.04	–	–	–	–	(4.3 ± 2.1) × 10 ⁻³	–
2-Cyclopentene-1,4-dione	C ₅ H ₄ O ₂	1089.66	2.389	0.012 ± 0.006	0.012 ± 0.006	–	(4.2 ± 2.1) × 10 ⁻³	(5.7 ± 2.8) × 10 ⁻³	–
1,4-Pentadien-3-one	C ₅ H ₆ O	499.846	2.592	–	(7.5 ± 3.8) × 10 ⁻⁴	–	–	(5.1 ± 2.6) × 10 ⁻³	–
3-Cyclopenten-1-one	C ₅ H ₈ O	694.784	3.37	(8.9 ± 4.4) × 10 ⁻³	0.015 ± 0.007	–	(2.7 ± 1.3) × 10 ⁻³	(3.9 ± 2.0) × 10 ⁻³	–
2-Cyclopenten-1-one	C ₅ H ₈ O	929.709	4.022	0.020 ± 0.01	0.063 ± 0.032	(7.0 ± 3.5) × 10 ⁻³	0.016 ± 0.008	0.062 ± 0.031	0.029 ± 0.015
3-Buten-2-one, 3-methyl-	C ₆ H ₁₀ O	479.853	1.888	0.029 ± 0.015	0.070 ± 0.035	(2.1 ± 1.0) × 10 ⁻³	0.011 ± 0.005	0.023 ± 0.012	0.035 ± 0.017
4-Penten-2-one	C ₆ H ₁₀ O	489.85	2.244	(2.2 ± 1.1) × 10 ⁻³	(4.1 ± 2.0) × 10 ⁻³	(2.3 ± 1.2) × 10 ⁻⁴	(4.9 ± 2.5) × 10 ⁻⁴	(2.5 ± 1.2) × 10 ⁻³	(2.1 ± 1.1) × 10 ⁻³
1-Penten-3-one	C ₆ H ₁₀ O	509.843	2.011	(2.5 ± 1.3) × 10 ⁻³	(3.4 ± 2.0) × 10 ⁻³	(6.1 ± 3.1) × 10 ⁻⁴	(1.2 ± 0.6) × 10 ⁻³	(8.4 ± 4.2) × 10 ⁻³	(2.7 ± 1.3) × 10 ⁻³
3-Penten-2-one (Z)	C ₆ H ₁₀ O	514.842	1.954	(2.0 ± 1.0) × 10 ⁻³	(4.3 ± 2.1) × 10 ⁻³	(2.4 ± 1.2) × 10 ⁻⁴	(5.7 ± 2.9) × 10 ⁻⁴	(3.9 ± 1.9) × 10 ⁻³	–
C ₆ H ₁₀ O isomer	C ₆ H ₁₀ O	609.811	2.244	–	–	–	–	(1.1 ± 0.6) × 10 ⁻³	–
3-Penten-2-one, (E)-	C ₆ H ₁₀ O	669.792	2.416	(7.7 ± 16.2) × 10 ⁻⁴	0.010 ± 0.005	(5.9 ± 2.9) × 10 ⁻⁴	(1.6 ± 0.8) × 10 ⁻³	0.014 ± 0.007	(5.0 ± 2.5) × 10 ⁻³
Cyclopentanone	C ₆ H ₁₀ O	799.75	2.583	0.011 ± 0.005	0.034 ± 0.017	(1.3 ± 0.7) × 10 ⁻³	(7.6 ± 3.8) × 10 ⁻³	0.025 ± 0.013	0.030 ± 0.015
2,3-Pentanedione	C ₆ H ₈ O ₂	534.835	2.178	(9.7 ± 4.9) × 10 ⁻³	0.026 ± 0.013	(6.0 ± 3.0) × 10 ⁻⁴	(6.9 ± 3.5) × 10 ⁻³	0.015 ± 0.008	(4.1 ± 2.0) × 10 ⁻³
2-Butanone, 3-methyl-	C ₆ H ₁₀ O	444.864	1.597	(6.3 ± 16.2) × 10 ⁻⁴	0.011 ± 0.006	(5.4 ± 2.7) × 10 ⁻⁴	(2.7 ± 1.4) × 10 ⁻³	(7.1 ± 3.5) × 10 ⁻³	0.050 ± 0.025
2-Pentanone									
C ₆ H ₁₀ O	509.843	1.734	(4.5 ± 1.6) × 10 ⁻³	0.019 ± 0.004	–	–	(2.3 ± 0.9) × 10 ⁻³	0.017 ± 0.003	0.016 ± 0.006
3-Pentanone	C ₆ H ₁₀ O	534.835	1.698	–	–	–	–	(6.3 ± 3.1) × 10 ⁻³	–
2,4-Hexadienal, (E,E)-	C ₆ H ₁₀ O	1034.68	3.045	–	–	–	–	(4.2 ± 2.1) × 10 ⁻³	–
2-Cyclopenten-1-one, 2-methyl-	C ₆ H ₁₀ O	1139.64	2.966	(6.0 ± 3.0) × 10 ⁻³	0.019 ± 0.009	(2.5 ± 1.3) × 10 ⁻³	(5.2 ± 2.6) × 10 ⁻³	0.026 ± 0.013	0.022 ± 0.011
2-Cyclohexen-1-one	C ₆ H ₈ O	1219.62	3.348	–	–	–	–	(2.4 ± 1.2) × 10 ⁻³	–
2-Cyclopenten-1-one, 3-methyl-	C ₆ H ₁₀ O	1314.59	3.762	–	–	–	–	(4.8 ± 2.4) × 10 ⁻³	–
2-Pentanone, 3-methylene-	C ₆ H ₁₀ O	734.771	1.817	–	–	–	–	(8.9 ± 4.5) × 10 ⁻⁴	–
1-Penten-3-one, 2-methyl-	C ₆ H ₁₀ O	749.766	1.773	–	–	–	–	(1.7 ± 0.8) × 10 ⁻³	–
5-Hexen-3-one	C ₆ H ₁₀ O	759.763	2.046	–	–	–	–	(4.6 ± 2.3) × 10 ⁻⁴	–
5-Hexen-2-one	C ₆ H ₁₀ O	759.763	2.138	–	(1.8 ± 1.4) × 10 ⁻³	–	–	(9.2 ± 4.6) × 10 ⁻⁴	–
1-Hexen-3-one	C ₆ H ₁₀ O	764.762	1.91	–	–	–	–	(5.8 ± 3.0) × 10 ⁻⁴	–
4-Hexen-2-one	C ₆ H ₁₀ O	789.754	1.83	–	–	–	–	(6.4 ± 3.2) × 10 ⁻⁴	–
4-Penten-2-one, 3-methyl-	C ₆ H ₁₀ O	834.739	2.134	–	(1.5 ± 1.4) × 10 ⁻³	–	–	–	–
2-Penten-2-one, 4-methyl-	C ₆ H ₁₀ O	838.738	1.984	–	–	–	–	(5.6 ± 2.8) × 10 ⁻⁴	–
4-Hexen-3-one isomer	C ₆ H ₁₀ O	859.731	2.187	–	–	–	–	(5.3 ± 2.6) × 10 ⁻⁴	–
4-Hexen-3-one isomer	C ₆ H ₁₀ O	939.706	2.121	–	–	–	–	(2.2 ± 1.1) × 10 ⁻³	–
Cyclopentanone, 2-methyl-	C ₆ H ₁₀ O	949.702	2.156	–	(8.1 ± 4.1) × 10 ⁻³	–	–	(7.9 ± 4.0) × 10 ⁻³	–
3-Penten-2-one, 3-methyl-	C ₆ H ₁₀ O	954.701	2.134	–	(1.2 ± 1.4) × 10 ⁻³	–	–	–	–
3-hexen-2-one	C ₆ H ₁₀ O	964.698	2.187	–	–	–	–	(10.0 ± 5.0) × 10 ⁻⁴	–
3-Methylcyclopentanone	C ₆ H ₁₀ O	974.694	2.248	–	–	–	–	(3.3 ± 1.6) × 10 ⁻³	–
Cyclohexanone									
C ₆ H ₁₀ O	1109.65	2.473	–	–	(6.9 ± 1.5) × 10 ⁻³	–	(1.6 ± 0.7) × 10 ⁻³	(1.7 ± 0.3) × 10 ⁻³	0.015 ± 0.004
C ₆ Diketone isomer	C ₆ H ₁₀ O ₂	664.794	1.738	–	–	–	–	–	(8.1 ± 6.0) × 10 ⁻³
C ₆ Diketone isomer	C ₆ H ₁₀ O ₂	789.754	1.976	(1.1 ± 0.5) × 10 ⁻³	–	(2.9 ± 4.1) × 10 ⁻⁴	(1.1 ± 0.6) × 10 ⁻³	(1.9 ± 1.0) × 10 ⁻³	–

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
						Giant Cutgrass	Wiregrass		
C ₆ Diketone isomer	C ₆ H ₁₀ O ₂	829.741	1.932	–	–	–	–	(6.2 ± 3.1) × 10 ⁻⁴	–
C ₆ Diketone isomer	C ₆ H ₁₀ O ₂	874.726	1.852	0.013 ± 0.006	(2.3 ± 1.4) × 10 ⁻³	–	–	(3.2 ± 1.6) × 10 ⁻³	(4.1 ± 4.0) × 10 ⁻³
Methyl Isobutyl Ketone	C ₆ H ₁₂ O	664.794	1.61	–	(4.3 ± 3.0) × 10 ⁻³	–	–	(9.5 ± 6.6) × 10 ⁻⁴	0.011 ± 0.009
3-Pentanone, 2-methyl-	C ₆ H ₁₂ O	689.786	1.536	–	–	–	–	(2.7 ± 3.0) × 10 ⁻⁴	(6.4 ± 3.2) × 10 ⁻³
2-Pentanone, 3-methyl-	C ₆ H ₁₂ O	699.782	1.61	–	–	–	–	(9.5 ± 4.7) × 10 ⁻⁴	0.020 ± 0.01
3-Hexanone	C ₆ H ₁₂ O	784.755	1.628	–	–	–	–	(2.0 ± 1.0) × 10 ⁻³	–
2-Hexanone	C ₆ H ₁₂ O	804.749	1.729	(2.6 ± 1.2) × 10 ⁻³	(5.7 ± 1.4) × 10 ⁻³	–	–	(2.6 ± 0.5) × 10 ⁻³	0.011 ± 0.004
Cyclopentanone, 3,4-bis(methylene)-	C ₇ H ₁₀ O	1289.59	2.873	–	–	–	–	(8.5 ± 4.3) × 10 ⁻⁴	–
2-Cyclopenten-1-one, 3,4-dimethyl-	C ₇ H ₁₀ O	1229.61	2.358	–	(4.1 ± 2.0) × 10 ⁻³	–	–	(4.5 ± 2.3) × 10 ⁻³	–
3-methyl-3-cyclohexen-1-one	C ₇ H ₁₀ O	1254.6	2.407	–	–	–	–	(1.8 ± 0.9) × 10 ⁻³	–
2-Cyclopenten-1-one, 2,3-dimethyl-	C ₇ H ₁₀ O	1389.56	2.618	–	–	–	–	(3.3 ± 1.6) × 10 ⁻³	–
C7H10O isomer	C ₇ H ₁₀ O	1514.52	2.917	–	–	–	–	(1.6 ± 0.8) × 10 ⁻³	–
Cyclopentanone, 2-ethyl-	C ₇ H ₁₂ O	1234.61	2.033	–	–	–	–	(9.4 ± 4.7) × 10 ⁻⁴	–
3-pentanone, 2,4-dimethyl	C ₇ H ₁₄ O	664.794	1.747	(5.3 ± 2.7) × 10 ⁻³	–	(3.4 ± 1.7) × 10 ⁻³	–	(1.5 ± 0.8) × 10 ⁻³	(8.0 ± 4.0) × 10 ⁻³
2-Heptanone	C ₇ H ₁₄ O	1094.66	1.694	–	(2.4 ± 1.4) × 10 ⁻³	–	–	(9.7 ± 4.8) × 10 ⁻⁴	(8.6 ± 4.3) × 10 ⁻³
Esters									
Acetic acid, methyl ester	C ₅ H ₈ O ₂	209.939	1.342	0.024 ± 0.012	0.047 ± 0.024	(6.4 ± 3.2) × 10 ⁻³	0.029 ± 0.014	–	0.080 ± 0.04
Acetic acid ethenyl ester	C ₅ H ₈ O ₂	279.917	1.619	(6.1 ± 3.1) × 10 ⁻³	(3.4 ± 1.7) × 10 ⁻³	–	–	–	–
Ethyl Acetate	C ₅ H ₈ O ₂	339.898	1.527	–	–	–	–	(5.3 ± 2.7) × 10 ⁻⁴	–
2-Propenoic acid, methyl ester	C ₅ H ₈ O ₂	344.896	1.817	(6.1 ± 3.1) × 10 ⁻³	(9.4 ± 4.7) × 10 ⁻³	–	(1.6 ± 0.8) × 10 ⁻³	(2.5 ± 1.2) × 10 ⁻³	(7.2 ± 3.6) × 10 ⁻³
Butyrolactone	C ₅ H ₈ O ₂	1159.64	2.68	–	(7.3 ± 3.7) × 10 ⁻³	(7.0 ± 3.5) × 10 ⁻⁴	–	0.015 ± 0.008	–
Acetic anhydride	C ₅ H ₈ O ₂	789.754	3.353	0.012 ± 0.006	0.018 ± 0.009	–	(2.7 ± 1.3) × 10 ⁻³	(7.4 ± 3.7) × 10 ⁻³	–
Methyl propionate	C ₅ H ₈ O ₂	369.888	1.571	(2.3 ± 1.1) × 10 ⁻³	(5.8 ± 2.9) × 10 ⁻³	–	(2.9 ± 1.4) × 10 ⁻³	(4.3 ± 2.2) × 10 ⁻³	(9.2 ± 4.6) × 10 ⁻³
2(3H)-Furanone, 5-methyl-	C ₅ H ₈ O ₂	1044.67	4.343	–	(3.1 ± 1.5) × 10 ⁻³	–	(7.6 ± 3.8) × 10 ⁻⁴	–	–
Acetic acid, 2-propenyl ester	C ₅ H ₈ O ₂	544.832	1.94	(3.6 ± 1.8) × 10 ⁻³	(3.8 ± 1.9) × 10 ⁻³	–	–	(1.1 ± 0.6) × 10 ⁻³	–
Methacrylic acid methyl ester	C ₅ H ₈ O ₂	579.821	1.716	(2.3 ± 1.1) × 10 ⁻³	(6.2 ± 3.1) × 10 ⁻³	–	–	–	–
2-Butenoic acid, methyl ester	C ₅ H ₈ O ₂	739.77	2.02	–	–	–	–	(7.6 ± 3.8) × 10 ⁻⁴	–
Butanoic acid, methyl ester	C ₅ H ₁₀ O ₂	604.813	1.584	–	(2.8 ± 1.4) × 10 ⁻³	–	(1.4 ± 0.7) × 10 ⁻³	(1.5 ± 0.8) × 10 ⁻³	–
2-Vinylethyl acetate	C ₆ H ₁₀ O ₂	814.746	1.839	(1.8 ± 0.9) × 10 ⁻³	–	–	–	–	–
Acetic acid, butyl ester	C ₆ H ₁₂ O ₂	869.728	1.549	–	(3.4 ± 1.7) × 10 ⁻³	–	–	–	–
Isobutyric acid, allyl ester	C ₇ H ₁₂ O ₂	979.693	4.25	–	–	(9.1 ± 4.5) × 10 ⁻⁴	–	–	–
Alcohols									
Isopropyl Alcohol	C ₃ H ₈ O	174.95	1.795	(2.6 ± 1.2) × 10 ⁻³	–	(4.8 ± 1.0) × 10 ⁻³	–	(7.5 ± 1.5) × 10 ⁻³	–
2-Propen-1-ol	C ₃ H ₆ O	219.936	4.255	0.016 ± 0.008	0.023 ± 0.012	(1.0 ± 0.5) × 10 ⁻³	(2.7 ± 1.3) × 10 ⁻³	(6.5 ± 3.3) × 10 ⁻³	–
1-Butanol	C ₄ H ₁₀ O	429.869	3.731	(7.0 ± 2.3) × 10 ⁻³	0.030 ± 0.021	(5.3 ± 1.1) × 10 ⁻³	0.018 ± 0.004	(5.8 ± 1.2) × 10 ⁻³	–
Other									
2H-Pyran, 3,4-dihydro-	C ₆ H ₈ O	514.842	1.54	(1.6 ± 0.9) × 10 ⁻³	(3.0 ± 1.5) × 10 ⁻³	–	(6.8 ± 4.8) × 10 ⁻⁴	–	–
Furans									
Furan	C ₄ H ₄ O	179.949	1.236	0.23 ± 0.05	0.31 ± 0.06	0.022 ± 0.004	0.065 ± 0.013	0.085 ± 0.017	0.31 ± 0.06
Furan, 2,5-dihydro-	C ₄ H ₆ O	259.923	1.91	(2.4 ± 2.0) × 10 ⁻³	(3.1 ± 2.5) × 10 ⁻³	–	–	(5.3 ± 2.7) × 10 ⁻⁴	–
2,3-Dihydrofuran	C ₄ H ₆ O	264.922	1.39	(9.9 ± 4.9) × 10 ⁻³	0.021 ± 0.01	–	0.011 ± 0.005	(5.9 ± 3.0) × 10 ⁻³	(6.1 ± 3.1) × 10 ⁻³
Furan, tetrahydro-	C ₄ H ₆ O	364.89	1.412	(1.8 ± 2.0) × 10 ⁻³	(3.2 ± 2.5) × 10 ⁻³	(5.4 ± 1.2) × 10 ⁻⁴	(5.8 ± 10.8) × 10 ⁻⁴	(1.4 ± 0.5) × 10 ⁻³	–
Furan, 2-methyl-	C ₅ H ₆ O	319.904	1.487	0.13 ± 0.03	0.21 ± 0.04	(8.6 ± 1.7) × 10 ⁻³	0.045 ± 0.009	0.066 ± 0.013	0.23 ± 0.05

23295

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
						Giant Cutgrass	Wiregrass		
Furan, 3-methyl-	C ₅ H ₆ O	334.899	1.575	0.013 ± 0.007	0.022 ± 0.011	(1.2 ± 0.6) × 10 ⁻³	(5.0 ± 2.5) × 10 ⁻³	(7.6 ± 3.8) × 10 ⁻³	0.025 ± 0.012
Furan, 2,3-dihydro-5-methyl-	C ₅ H ₆ O	459.859	1.456	(2.2 ± 1.1) × 10 ⁻³	(6.2 ± 3.1) × 10 ⁻³	–	(2.8 ± 1.4) × 10 ⁻³	(1.2 ± 0.6) × 10 ⁻³	–
Vinylfuran	C ₅ H ₆ O	619.808	2.09	(6.9 ± 3.4) × 10 ⁻³	(9.5 ± 4.8) × 10 ⁻³	(8.7 ± 4.4) × 10 ⁻⁴	(1.1 ± 1.2) × 10 ⁻³	(5.1 ± 2.5) × 10 ⁻³	–
Furan, 2-ethyl-	C ₆ H ₆ O	544.832	1.531	(6.9 ± 3.4) × 10 ⁻³	0.012 ± 0.006	(1.0 ± 0.5) × 10 ⁻³	(1.1 ± 1.2) × 10 ⁻³	(6.8 ± 3.4) × 10 ⁻³	0.012 ± 0.008
Furan, 2,5-dimethyl-	C ₆ H ₆ O	569.824	1.5	0.038 ± 0.008	0.079 ± 0.016	(8.7 ± 8.3) × 10 ⁻⁴	(8.8 ± 1.8) × 10 ⁻³	0.027 ± 0.005	0.066 ± 0.013
Furan, 3-ethyl-	C ₆ H ₆ O	579.821	1.637	(1.5 ± 0.8) × 10 ⁻³	(2.1 ± 1.1) × 10 ⁻³	–	(6.1 ± 3.0) × 10 ⁻⁴	(5.3 ± 6.0) × 10 ⁻⁴	–
Furan, 2,4-dimethyl-	C ₆ H ₆ O	594.816	1.54	(6.2 ± 3.1) × 10 ⁻³	0.013 ± 0.007	(6.7 ± 3.3) × 10 ⁻⁴	(2.0 ± 1.2) × 10 ⁻³	(3.7 ± 1.9) × 10 ⁻³	0.034 ± 0.017
Furan, 2,3-dimethyl-	C ₆ H ₆ O	599.814	1.553	–	–	–	–	(1.8 ± 0.9) × 10 ⁻⁴	–
Furan, 2-(1-propenyl)-	C ₇ H ₆ O	939.706	1.98	–	–	–	–	(6.4 ± 3.2) × 10 ⁻⁴	–
Furan, 2-(2-propenyl)-	C ₇ H ₆ O	1009.68	2.002	–	(2.9 ± 1.4) × 10 ⁻³	–	(6.9 ± 3.4) × 10 ⁻⁴	(9.0 ± 6.1) × 10 ⁻⁴	–
Furan, 2-propyl-	C ₇ H ₈ O	799.75	1.505	(9.8 ± 4.9) × 10 ⁻⁴	(2.0 ± 1.0) × 10 ⁻³	–	–	(3.7 ± 6.0) × 10 ⁻⁴	–
Furan, 2-ethyl-5-methyl-	C ₇ H ₈ O	829.741	1.452	(5.4 ± 2.7) × 10 ⁻³	0.010 ± 0.005	–	(0.9 ± 12.3) × 10 ⁻⁴	(6.0 ± 3.0) × 10 ⁻³	0.014 ± 0.008
Furan, 2,3,5-trimethyl-	C ₇ H ₈ O	889.722	1.474	(3.0 ± 1.5) × 10 ⁻³	(2.5 ± 2.8) × 10 ⁻³	–	(9.9 ± 4.9) × 10 ⁻⁴	(1.3 ± 0.7) × 10 ⁻³	(7.4 ± 8.0) × 10 ⁻³
2-Propionylfuran	C ₇ H ₈ O ₂	1429.55	3.555	–	–	–	–	(1.5 ± 0.8) × 10 ⁻³	–
Furan, 4-methyl-2-propyl-	C ₈ H ₁₀ O	1074.66	1.408	(9.8 ± 4.9) × 10 ⁻⁴	–	–	–	–	–
Aldehydes and Ketones									
3-Furaldehyde	C ₆ H ₄ O ₂	869.728	1.012	0.017 ± 0.008	0.029 ± 0.014	(2.5 ± 1.2) × 10 ⁻³	(8.5 ± 4.2) × 10 ⁻³	(9.5 ± 4.7) × 10 ⁻³	–
Furfural	C ₆ H ₄ O ₂	934.707	1.131	0.21 ± 0.04	0.44 ± 0.09	0.021 ± 0.004	0.16 ± 0.03	0.20 ± 0.04	0.35 ± 0.07
Furan, 2-acetyl-	C ₆ H ₆ O ₂	1164.63	4.484	(6.6 ± 3.3) × 10 ⁻³	0.018 ± 0.009	(2.1 ± 1.0) × 10 ⁻³	(6.0 ± 3.0) × 10 ⁻³	0.018 ± 0.009	–
5-methyl furfural	C ₆ H ₆ O ₂	1309.59	4.396	0.013 ± 0.003	0.034 ± 0.007	–	(7.2 ± 1.4) × 10 ⁻³	0.042 ± 0.008	0.051 ± 0.01
Methyl 2-furoate	C ₆ H ₆ O ₃	1344.58	4.088	–	–	–	–	(1.6 ± 0.8) × 10 ⁻³	–
2-Acetyl-5-methylfuran	C ₇ H ₆ O ₂	1509.52	3.542	–	–	–	–	(1.9 ± 1.0) × 10 ⁻³	–
Alcohols									
2-furan methanol	C ₅ H ₆ O ₂	984.691	3.309	0.043 ± 0.009	0.13 ± 0.03	0.010 ± 0.002	0.071 ± 0.014	0.12 ± 0.02	–
N- and S-Containing Compounds									
Nitriles									
Acetonitrile	C ₂ H ₃ N	169.952	2.592	0.018 ± 0.004	0.031 ± 0.006	0.021 ± 0.004	–	0.021 ± 0.004	0.064 ± 0.013
Acrylonitrile	C ₃ H ₃ N	199.942	2.433	0.018 ± 0.004	0.031 ± 0.006	0.020 ± 0.004	(1.6 ± 0.7) × 10 ⁻³	(9.5 ± 1.9) × 10 ⁻³	0.018 ± 0.005
Propanenitrile	C ₃ H ₃ N	269.92	2.873	(9.8 ± 4.9) × 10 ⁻³	0.018 ± 0.009	(5.9 ± 2.9) × 10 ⁻³	(1.3 ± 0.7) × 10 ⁻³	(9.1 ± 4.5) × 10 ⁻³	0.024 ± 0.012
Methacrylonitrile	C ₄ H ₃ N	309.907	2.306	(7.5 ± 1.5) × 10 ⁻³	0.011 ± 0.002	(4.1 ± 0.8) × 10 ⁻³	–	(5.1 ± 1.0) × 10 ⁻³	0.013 ± 0.004
3-Butenenitrile	C ₄ H ₃ N	409.875	3.221	(4.2 ± 2.1) × 10 ⁻³	(8.0 ± 4.0) × 10 ⁻³	(3.0 ± 1.5) × 10 ⁻³	–	(3.6 ± 1.8) × 10 ⁻³	–
2-Butenenitrile	C ₄ H ₃ N	494.848	3.705	–	(5.6 ± 2.8) × 10 ⁻³	(2.2 ± 1.1) × 10 ⁻³	–	(2.6 ± 1.3) × 10 ⁻³	–
Isobutyronitrile	C ₄ H ₃ N	359.891	2.332	(5.8 ± 2.9) × 10 ⁻³	(9.3 ± 4.6) × 10 ⁻³	(2.4 ± 1.2) × 10 ⁻³	–	(4.0 ± 2.0) × 10 ⁻³	0.018 ± 0.009
Butanenitrile	C ₄ H ₃ N	464.858	2.988	(3.7 ± 1.9) × 10 ⁻³	(5.2 ± 2.6) × 10 ⁻³	(1.4 ± 0.7) × 10 ⁻³	–	(2.7 ± 1.3) × 10 ⁻³	0.013 ± 0.006
2,4-Pentadienenitrile	C ₅ H ₃ N	684.787	4.176	–	–	(1.1 ± 0.5) × 10 ⁻³	–	–	–
Butanenitrile, 2-methylen-	C ₅ H ₃ N	614.81	2.319	–	–	–	–	(1.3 ± 0.6) × 10 ⁻³	–
3-Butenenitrile, 3-methyl-	C ₅ H ₃ N	759.763	3.106	–	–	–	–	(1.4 ± 0.7) × 10 ⁻³	–
Butanenitrile, 2-methyl-	C ₅ H ₃ N	609.811	2.288	(4.4 ± 2.2) × 10 ⁻³	(6.0 ± 3.0) × 10 ⁻³	(1.3 ± 0.7) × 10 ⁻³	–	(2.0 ± 1.0) × 10 ⁻³	0.016 ± 0.008
Butanenitrile, 3-methyl-	C ₅ H ₃ N	624.806	2.583	(5.9 ± 2.9) × 10 ⁻³	(1.0 ± 1.0) × 0.005	(2.2 ± 1.1) × 10 ⁻³	–	(4.8 ± 2.4) × 10 ⁻³	0.019 ± 0.009
Pentanenitrile	C ₅ H ₃ N	754.765	2.794	–	–	–	–	(1.0 ± 0.5) × 10 ⁻³	–
Pentanenitrile, 4-methyl-	C ₆ H ₃ N	954.701	2.486	(3.8 ± 1.9) × 10 ⁻³	(5.7 ± 2.9) × 10 ⁻³	(1.5 ± 0.7) × 10 ⁻³	–	(2.7 ± 1.4) × 10 ⁻³	–
Benzonitrile	C ₆ H ₃ N	1369.57	4.541	0.017 ± 0.003	0.026 ± 0.005	0.037 ± 0.007	(4.5 ± 1.4) × 10 ⁻³	0.013 ± 0.003	0.064 ± 0.013
Benzonitrile, 3-methyl-	C ₇ H ₃ N	1599.49	3.577	–	–	(2.5 ± 1.3) × 10 ⁻³	–	–	–

Table A1. Continued.

Compound	Formula	Prim. RT (s)	Sec. RT (s)	Black Spruce	Ponderosa Pine	Emission Factors (g kg ⁻¹)		Rice Straw	Indonesian Peat
						Giant Cutgrass	Wiregrass		
Pyroles									
Pyrrole	C ₄ H ₄ N	694.784	4.602	0.042 ± 0.008	0.11 ± 0.02	0.023 ± 0.005	0.014 ± 0.003	0.050 ± 0.01	0.055 ± 0.011
1H-Pyrrole, 1-methyl-	C ₅ H ₅ N	664.794	2.574	0.011 ± 0.005	0.021 ± 0.011	(2.3 ± 1.2) × 10 ⁻³	(4.1 ± 2.0) × 10 ⁻³	(5.7 ± 2.9) × 10 ⁻³	0.031 ± 0.016
1H-Pyrrole, 2-methyl-	C ₆ H ₆ N	934.707	4.167	(4.9 ± 3.1) × 10 ⁻³	0.015 ± 0.008	(2.3 ± 1.1) × 10 ⁻³	—	(6.8 ± 3.4) × 10 ⁻³	0.018 ± 0.011
1H-Pyrrole, 3-methyl-	C ₆ H ₆ N	959.699	4.294	—	(5.4 ± 3.7) × 10 ⁻³	—	—	(3.8 ± 1.9) × 10 ⁻³	—
1H-Pyrrole, 1-ethyl-	C ₆ H ₆ N	874.726	2.235	—	(6.2 ± 3.7) × 10 ⁻³	—	—	(1.6 ± 0.8) × 10 ⁻³	—
1H-Pyrrole, 2,4-dimethyl-	C ₈ H ₈ N	949.702	2.218	—	—	—	—	(1.4 ± 0.8) × 10 ⁻³	—
1H-Pyrrole, 2,5-dimethyl-	C ₈ H ₈ N	1044.67	2.398	—	(5.9 ± 3.7) × 10 ⁻³	—	—	(1.2 ± 0.8) × 10 ⁻³	0.014 ± 0.011
1H-Pyrrole, 2-ethyl-	C ₈ H ₈ N	1174.63	1.822	—	—	—	—	(1.1 ± 0.8) × 10 ⁻³	—
Pyridines									
Pyridine	C ₅ H ₅ N	674.79	2.992	0.014 ± 0.003	0.030 ± 0.006	0.022 ± 0.004	(4.2 ± 0.9) × 10 ⁻³	0.019 ± 0.004	0.12 ± 0.02
Pyridine, 2-methyl-	C ₆ H ₇ N	889.722	2.442	—	(5.8 ± 2.9) × 10 ⁻³	(2.0 ± 1.0) × 10 ⁻³	—	(6.1 ± 3.0) × 10 ⁻³	0.020 ± 0.01
Pyridine, 3-methyl-	C ₆ H ₇ N	1024.68	2.684	—	—	—	—	(2.4 ± 1.2) × 10 ⁻³	—
Thiophenes									
Thiophene	C ₄ H ₄ S	464.858	2.174	(3.6 ± 1.0) × 10 ⁻³	(4.6 ± 1.2) × 10 ⁻³	(6.9 ± 1.4) × 10 ⁻³	—	(2.6 ± 0.5) × 10 ⁻³	0.010 ± 0.004
Thiophene, 2-methyl-	C ₅ H ₆ S	754.765	1.954	—	(1.9 ± 1.2) × 10 ⁻³	—	—	(7.9 ± 4.0) × 10 ⁻⁴	(6.7 ± 3.5) × 10 ⁻³
Thiophene, 3-methyl-	C ₅ H ₆ S	779.757	2.064	—	—	—	—	(6.1 ± 3.0) × 10 ⁻⁴	—
Benzo[a]thiophene	C ₈ H ₆ S	1914.39	3.428	—	—	(3.6 ± 0.7) × 10 ⁻³	—	—	—
Other									
Pyrazine	C ₄ H ₄ N ₂	629.805	3.665	—	—	—	—	(2.9 ± 1.4) × 10 ⁻³	—
Pyrazine, methyl-	C ₅ H ₆ N ₂	904.717	2.86	—	—	—	—	(3.4 ± 1.7) × 10 ⁻³	—
3-Methylpyridazine	C ₅ H ₆ N ₂	1074.66	3.863	(7.1 ± 3.5) × 10 ⁻³	0.013 ± 0.007	—	—	(5.9 ± 3.0) × 10 ⁻³	—
Total Emission Factor				8.21 ± 2.45	11.43 ± 3.4	1.42 ± 0.36	1.08 ± 0.32	3.36 ± 1.01	14.58 ± 4.29
# Positively Identified				127	164	64	64	118	126
# Tentatively Identified				275	334	80	65	274	241
Total # of Compounds Identified				402	474	148	129	392	367
Percent Positively Identified				32%	30%	46%	50%	30%	34%

N/A = Not available

23297

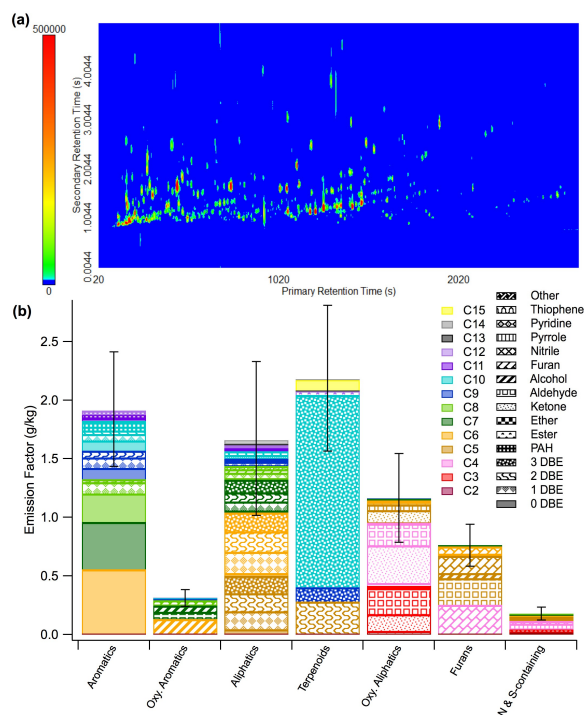


Figure 1. (a) GC \times GC/TOFMS chromatogram of NMOC emissions from a black spruce fire. The colorscale saturates at 500 000 A.U. **(b)** Summary of the compounds observed by GC \times GC/TOFMS during the black spruce fire. Colors indicate carbon number and patterns indicate functionality. ("DBE" = Double Bond Equivalents, which for aromatic compounds refers to the substituents only.)

23298

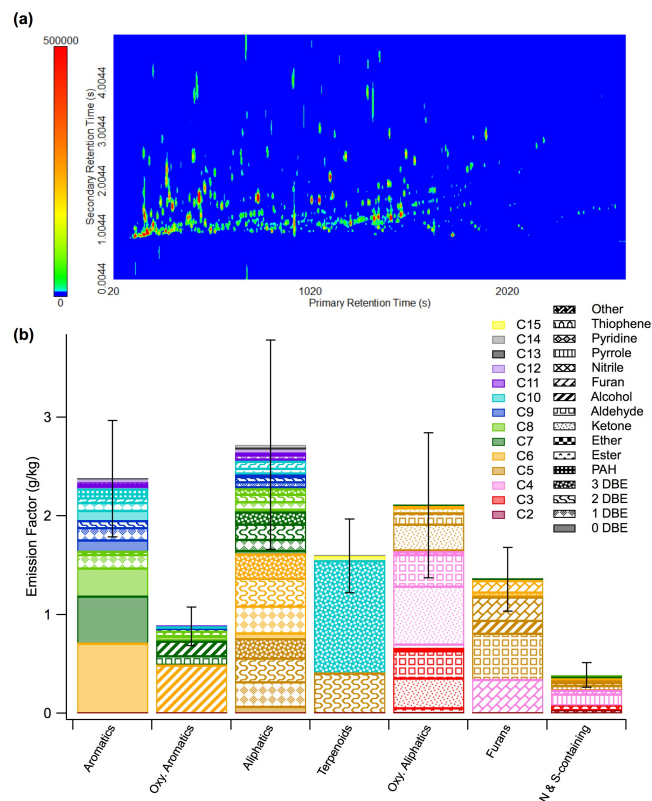


Figure 2. As in Fig. 1, for a ponderosa pine fire.

23299

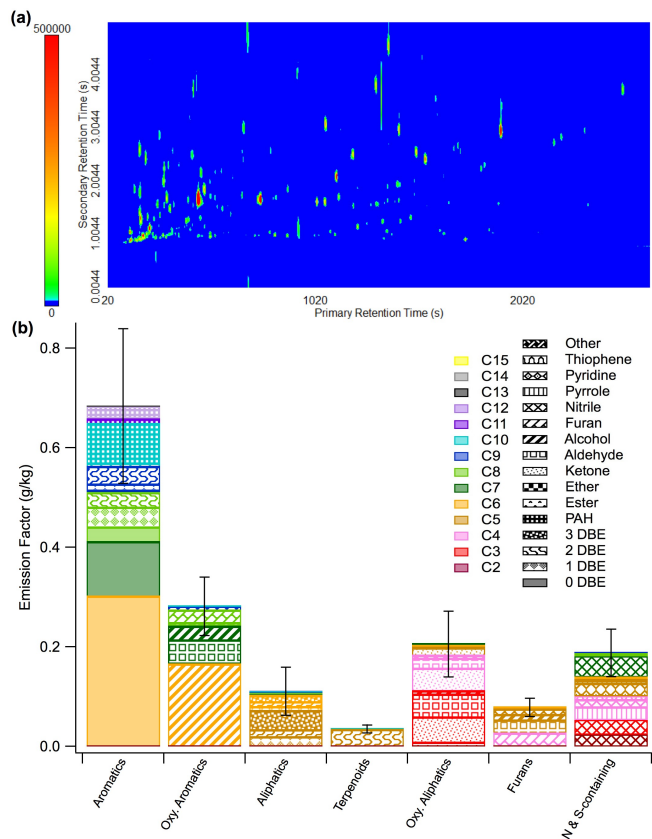


Figure 3. As in Fig. 1, for a giant cutgrass fire.

23300

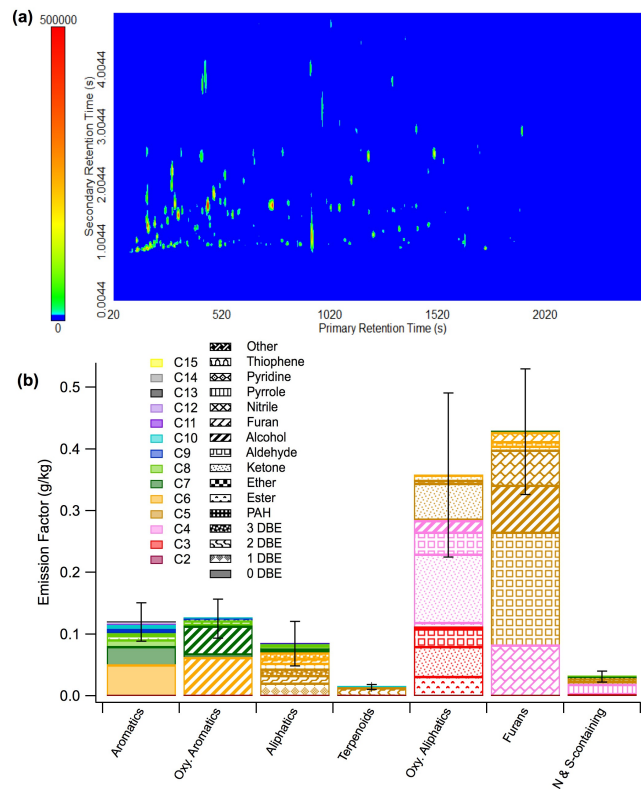


Figure 4. As in Fig. 1, for a wiregrass fire.

23301

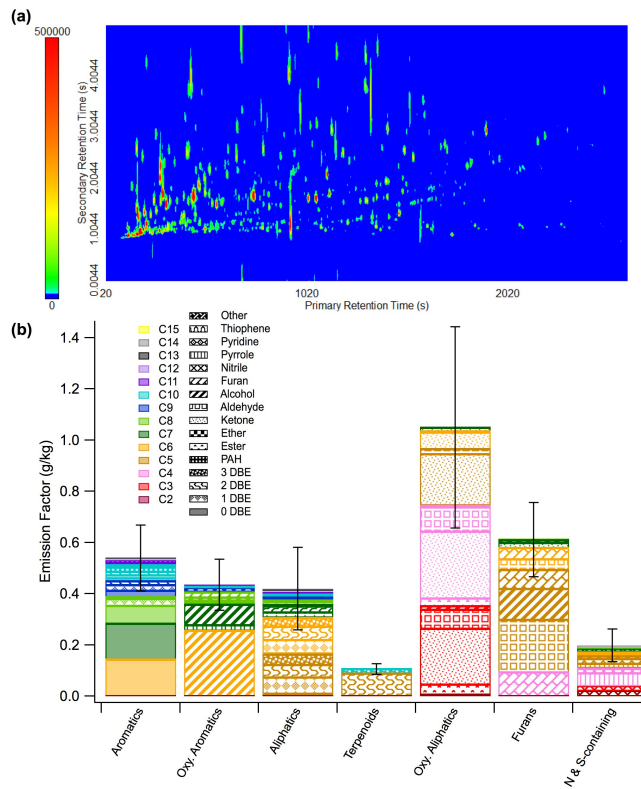


Figure 5. As in Fig. 1, for a Chinese rice straw fire.

23302

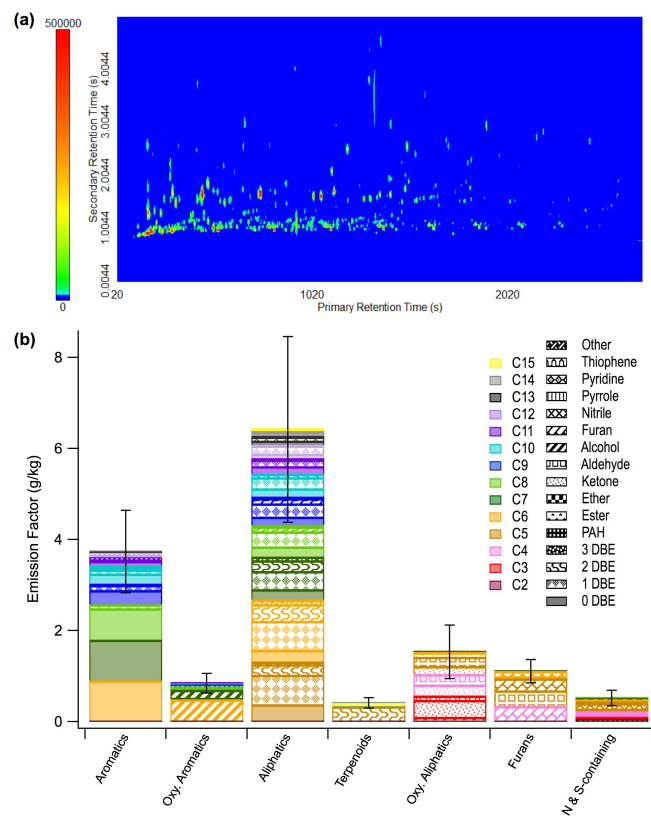


Figure 6. As in Fig. 1, for an Indonesian peat fire.

23303

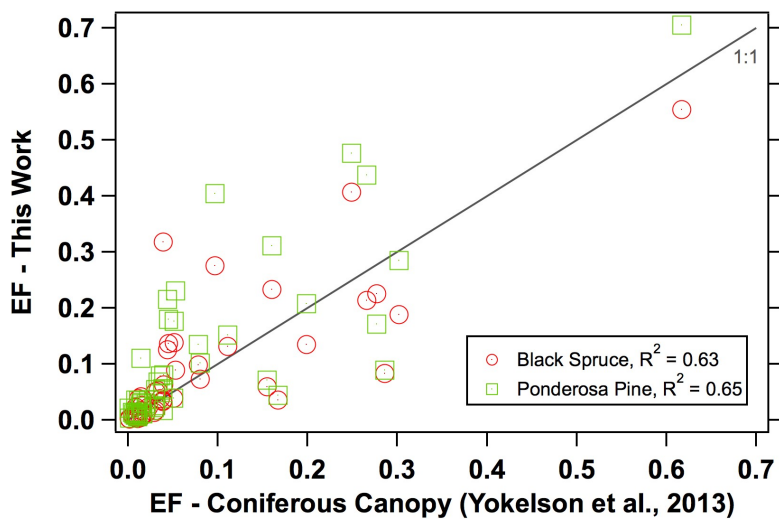


Figure 7. Comparison of the EFs measured for BS and PP, compared to the average of coniferous canopy burns given by Yokelson et al. (2013).

23304

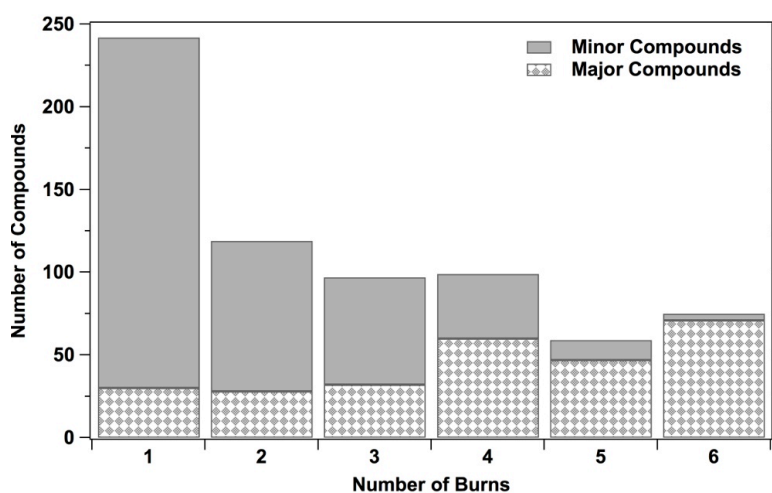


Figure 8. Histogram of the number of compounds present in the indicated number of burns. Compounds were considered “Major” if the EF was $> 0.01 \text{ g kg}^{-1}$ in any burn. All other compounds were classified as “Minor”.

23305

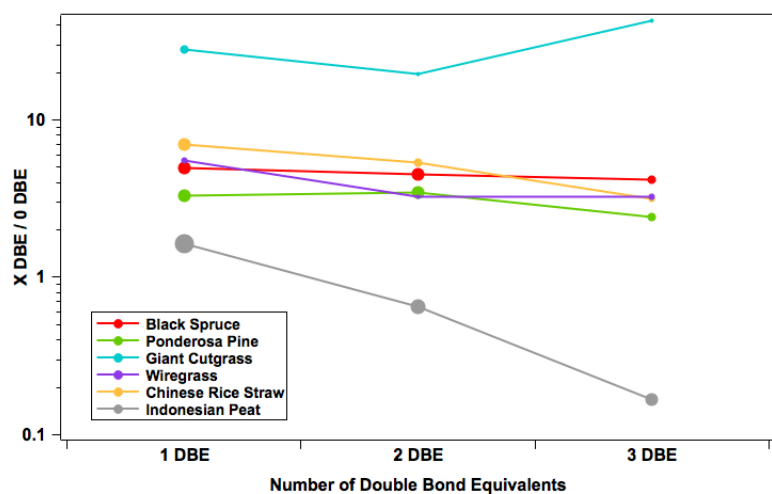


Figure 9. Ratio of the EFs for unsaturated aliphatic hydrocarbons (separated by double bond equivalents, DBE) vs. alkanes. The marker sizes are proportional to the average carbon number (from 5 to 8) at each DBE.

23306

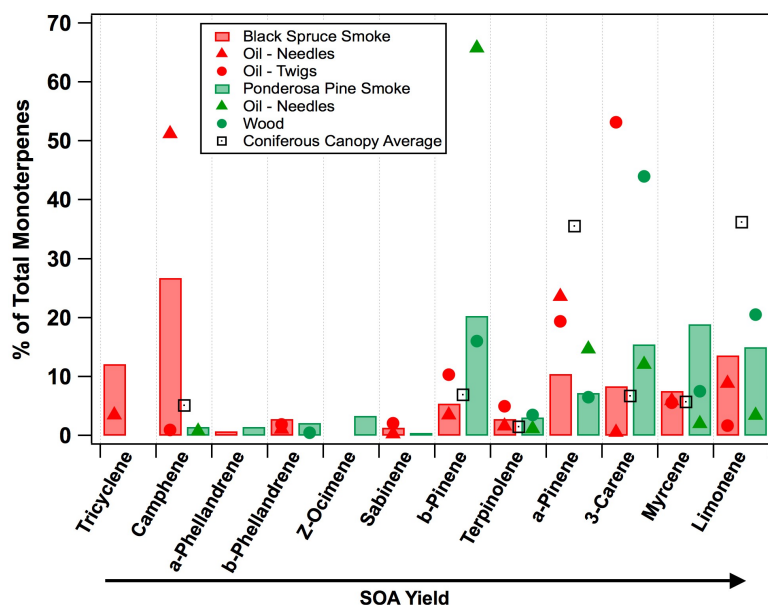


Figure 10. Distribution of the monoterpene isomers observed in smoke from fires of black spruce and ponderosa pine, as a percentage of the total monoterpene emission factor. The compounds are sorted in order of increasing SOA yield, largely based on Lee et al. (2006). Colored markers represent the percentage of each monoterpene measured in the essential oils of black spruce needles and twigs (von Rudloff, 1975) and ponderosa pine needles (Krauze-Baranowska et al., 2002) and wood (Anderson et al., 1969). Black squares indicate the MT emissions averaged over “Coniferous Canopy” fires reported in (Yokelson et al., 2013). All literature values were converted to % of reported monoterpenes.