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Introducing Volatile Organic Compound Model Intercomparison Project (VOCMIP)

Gunnar Myhre[1], Øivind Hodnebrog[1], Srinath Krishnan[1], Maria Sand[1], Marit Sandstad[1], Ragnhild B. Skeie[1], Lieven Clarisse[2], Bruno Franco[2], Dylan B. Millet[3], Kelley C. Wells[3], Alexander Archibald[4,5], Hannah N. Bryant[6], Alex T. Chaudhri[6], David S. Stevenson[6], Didier Hauglustaine[7], Michael Prather[8], J. Christopher Kaiser[9], Dirk J.L. Olivie[10], Michael Schulz[10], Oliver Wild[11], Ye Wang[11], Thérèse Salameh[12], Jason E. Williams[13], Philippe Le Sager[13], Fabien Paulot[14], Kostas Tsigaridis[15,16], Haley E. Plaas[15,16]

[1]CICERO Center for International Climate Research, 0318 Oslo, Norway
[2]Spectroscopy, Quantum Chemistry and Atmospheric Remote Sensing (SQUARES), BLU-ULB Research Centre, Université Libre de Bruxelles (ULB), 1050 Brussels, Belgium
[3]University of Minnesota, St. Paul, MN, 55108, USA.
[4]Yusuf Hamied Department of Chemistry, University of Cambridge, UK.
[5]National Centre for Atmospheric Science, UK.
[6]School of GeoSciences, The University of Edinburgh, EH9 3FF, UK
[7]Laboratoire des Sciences du Climat et de l'Environnement (LSCE), CEA/CNRS/UVSQ, IPSL, Université Paris-Saclay, Gif-sur-Yvette, France
[8]Earth System Science Department, University of California Irvine, Irvine, CA, USA
[9]Deutsches Zentrum für Luft- und Raumfahrt, Institut für Physik der Atmosphäre, Oberpfaffenhofen, Germany
[10]Norwegian Meteorological Institute, Oslo, Norway
[11]Lancaster Environment Centre, Lancaster University, Lancaster, LA1 4YQ, UK
[12]IMT Nord Europe, Institut Mines-Télécom, Univ. Lille, Centre for Energy and Environment, F-59000, Lille -France
[13]R&D Weather and Climate Modeling, Royal Netherlands Meteorological Institute, De Bilt, the Netherlands
[14]NOAA Geophysical Fluid Dynamics Laboratory, Princeton, NJ, USA
[15]Center for Climate Systems Research, Columbia University, New York, NY, USA
[16]NASA Goddard Institute for Space Studies, New York, NY, USA

Correspondence to: Gunnar Myhre (gunnar.myhre@cicero.oslo.no)

Abstract. Volatile organic compounds (VOCs) play an important role in atmospheric chemistry, influencing the cycling of peroxy and hydroxyl radicals, the formation of tropospheric ozone, hydrogen, secondary organic aerosol, and the lifetime of methane and other greenhouse gases. Their interactions shape overall atmospheric composition and air quality, with implications for both climate and human health. Given their significance, accurate representation of VOCs in global atmospheric chemistry models is crucial. In this context, we introduce the Volatile Organic Compound Model Intercomparison Project (VOCMIP) and invite atmospheric chemistry modelling groups to participate in this collaborative effort. VOCMIP aims to identify model consistencies and discrepancies, enhance the formulation of chemical mechanisms, and advance our understanding of VOC-related processes in the atmosphere. Global atmospheric chemistry model output will be compared to *in situ* measurements from surface stations and aircraft campaigns, plus satellite data for key VOCs. Special emphasis will be placed on formaldehyde (HCHO), examining its chemical sources and sinks given its central role as a radical source and as an intermediate in the photochemical destruction of VOCs.

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1 Introduction

Volatile organic compounds (VOCs) play a crucial role in atmospheric chemistry, acting as precursors to ozone (O_3) and influencing the lifetime of methane through competing reactions with hydroxyl radicals (OH). The direct greenhouse effect of VOCs is generally minor due to either low abundance or weak absorption of infrared radiation, but they can exert larger indirect climate effects through their influence on key atmospheric processes. VOCs consist of a large number of chemical species including hydrocarbons, oxygenated species, aromatics, organonitrates, halogenated VOCs, organosulfur compounds, multifunctional compounds (Goldstein and Galbally, 2007; Glasius and Goldstein, 2016; Mcdonald et al., 2018; Atkinson and Arey, 2003). Many VOCs are emitted into the atmosphere from primary natural and anthropogenic sources, some are formed in the atmosphere through secondary chemical reactions, and some have both primary and secondary sources. Key natural sources include biogenic emissions from vegetation (Guenther et al., 1995), marine emission (Yu and Li, 2021), while anthropogenic sources include industrial activities and transportation (Hoesly et al., 2018). Biomass burning emissions of VOCs (Van Marle et al., 2017) have both natural and anthropogenic sources. Additionally, volatile chemical products (VCPs), such as cosmetics, cleaners, and paints have gained increasing attention as a significant source of urban VOC emissions (Seltzer et al., 2021).

Observations and model simulations over North America suggest that a relatively small set of VOCs—including acetone, methanol, ethane, acetaldehyde, formaldehyde, isoprene, and methyl hydroperoxide—account for the majority of total atmospheric VOC abundance (Chen et al., 2019). Several studies have provided critical insights into the atmospheric budget of these individual VOCs, including methanol (Bates et al., 2021; Jacob et al., 2005; Wells et al., 2014), acetone (Wang et al., 2020; Khan et al., 2015b; Rivera et al., 2024), formaldehyde (Hoque et al., 2024; Luecken et al., 2018; Anderson et al., 2017), and methyl hydroperoxide (MHP) (Zhang et al., 2012). MHP plays a crucial role in regulating the tropospheric oxidizing capacity because it serves as a reservoir for HOx (the sum of OH and hydroperoxy, HO_2, radicals), a key driver of atmospheric chemistry (Allen et al., 2022; Khan et al., 2015a; Zhang et al., 2012). Isoprene, which is the most emitted biogenic VOC, has significant uncertainties from both its emissions (Dimaria et al., 2023; Messina et al., 2016; Guenther et al., 1995) and its oxidation chemistry (e.g.Bates and Jacob, 2019). The alkanes, ethane and propane, also come from direct sources, such as fossil fuel extraction, biomass burning, and natural gas usage (Blake and Rowland, 1995; Rosado-Reyes and Francisco, 2007; Rudolph, 1995). Atmospheric modelling studies often indicate that alkane emissions are underestimated (Dalsøren et al., 2018; Rowlinson et al., 2024), but model-measurement comparisons across Europe showed a good match for the spatial and temporal variations of major alkanes, including ethane (Ge et al., 2024). Broader assessments of multiple VOCs, such as the study by Safieddine et al. (2017), have advanced understanding of VOC interactions in the atmosphere. Nonetheless, inconsistencies in model representations of VOC sources, sinks, and chemical processes persist, underscoring the need for a coordinated effort to address these gaps (Ervens et al., 2024; Pozzer et al., 2007).

VOC's influence on ozone formation is complex (Sillman, 1999; Thornhill et al., 2021; Archibald et al., 2020b). In the presence of nitrogen oxides (NO_x), the photochemical oxidation of VOCs leads to the formation of ozone, impacting both air quality

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and climate. In the absence of NO_x, VOC oxidation leads to the destruction of O_3 through promotion of chain-terminating HO_x chemistry. Additionally, oxidation of VOCs generates low-volatility products that contribute to secondary organic aerosol (SOA) formation (Jimenez et al., 2009; Hallquist et al., 2009). These oxidation products can condense onto existing aerosol particles or nucleate new particles, impacting air quality, visibility, and climate by altering the Earth's radiative balance. The atmospheric oxidation of almost all VOCs results in the production of formaldehyde (HCHO) as a short-lived intermediate species. HCHO is destroyed through reaction with OH and photolysis (roughly 25% and 75%, respectively), with about 60% of the photolysis pathway leading to molecular hydrogen (H_2) and providing the principal atmospheric source of that molecule (Ehhalt and Rohrer, 2009). Accurately modeling formaldehyde's atmospheric budget is necessary for calculating hydrogen's indirect climate effects (Sand et al., 2023). Despite the complex atmospheric chemistry related to formaldehyde, Figure 1 highlights the primary species that contribute to formaldehyde formation (Nussbaumer et al., 2021), emphasizing the critical roles of natural emissions, anthropogenic emissions, and in situ chemical production, in the production of atmospheric formaldehyde. As such, to understand model differences in formaldehyde, we clearly need to examine a broad set of VOCs.

VOC oxidation chemistry is a central component of the chemical mechanisms in global atmospheric models. VOC oxidation is complex and explicit treatment of the oxidation steps from emitted VOC to final oxidation products (H_2O plus CO_2) can lead to 100,000s of reactions for even moderate size VOCs (Aumont et al., 2005). To reduce the complexity of the problem modellers employ two strategies: (1) select a subset of the dominant VOCs being emitted; and/or (2) reduce the complexity of the VOC oxidation mechanism by skipping intermediate steps. A common strategy is to lump a set of VOCs with similar reactivity against OH or O_3, and then select a surrogate VOC among that group for the chemical mechanism. All VOC emissions within that group are then emitted as the surrogate. As a variant, the OH reactivities (the rate constants for the reaction of OH with a VOC) of the individual VOCs in the group are used to scale their emissions to the surrogate species, thus conserving reactivity in the near field. When lumping VOC emissions, there is the option of conserving mass, carbon, or moles. For example, in the UKCA model's 'CheST' chemical scheme (Archibald et al., 2020a), ethane represents the total emitted mass of ethane, ethene and ethyne. Several studies have focused on understanding the impacts of these approaches in the past using box models (Derwent, 2020) or global atmospheric chemistry models (Archer-Nicholls et al., 2021; Utembe et al., 2010). All of these approximations produce biases in the near or far field chemistry and need to be tested with VOCMIP.

Given the significant diversity in how models represent VOCs, ranging from chemical scheme complexity, uncertainties in natural emissions, and scaling/grouping of VOC emissions, a coordinated intercomparison exercise is essential. Further, retrieval advancements for InfraRed (IR) satellite instruments like the Infrared Atmospheric Sounding Interferometer (IASI) (Franco et al., 2018) and the Cross-track Infrared Sounder (CrIS) (Wells et al., 2020) now provide valuable datasets for a wide range of VOCs, including methanol, acetone, and other key species. These datasets, which offer near-global, daily distributions of VOC vertical abundances in the atmosphere, present unprecedented opportunities to constrain the global budgets of VOCs. This adds to existing satellite retrievals of formaldehyde which have been available for several decades from various Ultraviolet-Visible (UV-Vis) satellite instruments (Burrows et al., 1999; De Smedt et al., 2021; Nowlan et al., 2023). Another,

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complementary valuable resource of VOC observations is the growing number of intensive aircraft campaigns in which multiple VOCs plus other reactive chemicals are measured over relatively small scales (e.g., 80 m x 2 km for 10s measurements) to map the spatial variability in VOCs (e.g. KORUS-AQ and ATom).

Here, we introduce the Volatile Organic Compound Model Intercomparison Project (VOCMIP) and invite atmospheric chemistry modelling groups to participate in this collaborative effort. VOCMIP seeks to identify commonalities and discrepancies, identify weaknesses in parameterizations, and improve our understanding of VOC-related processes in the atmosphere.

Methane is the most abundant VOC in the atmosphere and the dominant source of key VOCs like HCHO and methanol. In VOCMIP, however, methane is not a major focus and we will prescribe its lower boundary condition as a function of latitude based on observations.

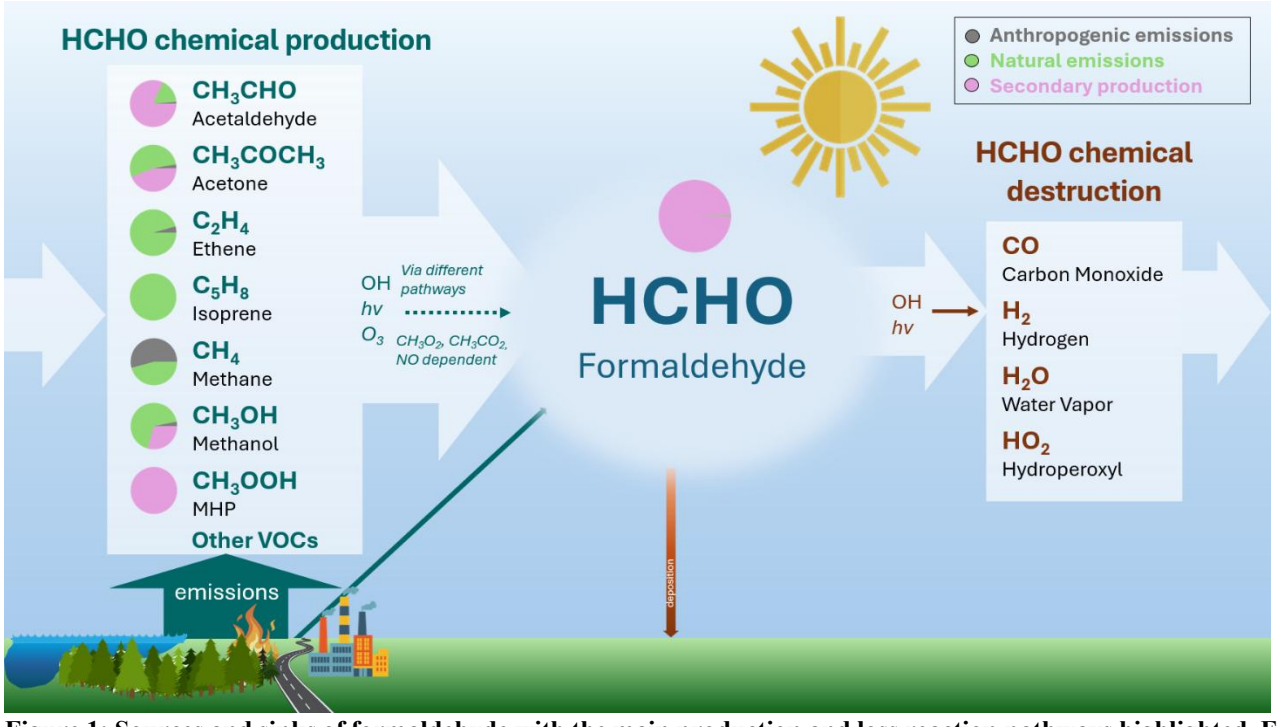

Figure 1: Sources and sinks of formaldehyde with the main production and loss reaction pathways highlighted. For the VOCs, the relative contributions from direct anthropogenic (grey), natural (green) emissions and secondary production in the atmosphere (pink) are presented as a pie-chart. These fractions are taken from various sources: acetaldehyde (CH_3CHO) from Millet et al. (2010), acetone (CH_3COCH_3) from Wang et al. (2020), ethene (C_2H_4) from CEDS (Hoesly et al., 2018) and MEGAN (Sindelarova et al., 2014) emissions, isoprene (C_5H_8) only includes natural emissions, methane (CH_4) from Jackson et al. (2024), methanol (CH_3OH) from Bates et al. (2021), MHP has only secondary production, formaldehyde (HCHO) stems from a OsloCTM3 simulation with CEDS, GFED4 (Van Der Werf et al., 2017) and MEGAN emissions, but direct BB emissions are <1% of the budget.

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2 Experimental design

We propose a set of model simulations for the selected years 2015 and 2019 (with years 2016-2018 as tier 2) with a necessary spinup period beginning 1 Jul 2014. We want the models to be run with the meteorology specific to those years to allow for
130 better comparison across models and with observations. Simulations should utilize meteorological fields from reanalysis, either nudged or directly prescribed as input to ensure consistency across models and to be representative of observed conditions. Anthropogenic emissions will be based on Community Emissions Data System (CEDS, version 2021) and biomass burning from GFEDv4 (Version 4.1), supplemented with natural emissions (e.g., MEGAN) as defined for each participating model.

The model output should include a comprehensive range of chemical compounds and other trace gases, or physical quantities
135 as outlined in Table 1. This output should be generated as single variable instantaneous 3-hourly 3D fields to capture satellite overpasses and temporal variations required for comparison to *in situ* measurements.

Table 2 provides a list of monthly mean budget terms required, using formaldehyde as an illustrative example. Emissions are requested for all emitted species listed in Table 1, while the additional budget terms are required for those VOCs (except propane and propene) listed in Table 1 in addition to hydrogen.

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Table 1: 3-hourly instantaneous 3d variables. Unit for airmass is kg m^{-2} and unit for all chemical compounds are mole $mole^{-1}$ of the compound relative to dry air. Nmvoc denotes the total of all non-methane VOCs included in the models including VOCs listed in the table. In addition, we request a more typical 3D monthly mean of these quantities and some standard model output*.

CF standard name	Chemical formula	Output variable name
atmosphere_mass_of_dryair_per_unit_area	Vertically integrated mass content of air in layer	airmass
mole_fraction_of_hydroxyl_radical_in_air	OH	oh
mole_fraction_of_ozone_in_air	O_3	o3
mole_fraction_of_carbon_monoxide_in_air	CO	co
mole_fraction_of_molecular_hydrogen_in_air	H_2	h2
mole_fraction_of_methane_in_air	CH_4	ch4
mole_fraction_of_ammonia_in_air	NH_3	nh3
mole_fraction_of_nitric oxide_in_air	NO	no
mole_fraction_of_nitrogen_dioxide_in_air	NO_2	no2
mole_fraction_of_nitric_acid_in_air	HNO_3	hno3
mole_fraction_of_peroxyacetylnitrate_in_air	$CH_3COO_2NO_2$	pan
mole_fraction_of_acetaldehyde_in_air	CH_3CHO	ch3cho

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mole_fraction_of_acetone_in_air	CH_3COCH_3	ch3coch3
mole_fraction_of_acetic_acid_in_air	CH_3COOH	ch3cooh
mole_fraction_of_benzene_in_air	C_6H_6	c6h6
mole_fraction_of_ethane_in_air	C_2H_6	c2h6
mole_fraction_of_ethene_in_air	C_2H_4	c2h4
mole_fraction_of_ethyne_in_air	C_2H_2	c2h2
mole_fraction_of_formaldehyde_in_air	HCHO	hcho
mole_fraction_of_formic_acid_in_air	HCOOH	hcooh
mole_fraction_of_glyoxal_in_air	CHOCHO	chocho
mole_fraction_of_isoprene_in_air	C_5H_8	isop
mole_fraction_of_methanol_in_air	CH_3OH	ch3oh
mole_fraction_of_mhp_in_air	CH_3OOH	mhp
mole_fraction_of_monoterpenes_in_air	$C_{10}H_{16}$	mtp
mole_fraction_of_propane_in_air	C_3H_8	c3h8
mole_fraction_of_propene_in_air	C_3H_6	c3h6
mole_fraction_of_nmvoc_expressed_as_carbon_in_air	NMVOC	nmvoc

*Standard model output of area of each grid cell and vertical layers is also required.

Table 2: Monthly 2d and 3d budget terms with formaldehyde as an example. Budget terms are required for every VOC (except propane and propene) listed in Table 1 in addition to hydrogen using the following approach: column integrated emissions to provide a 2D emissions field (emi_x). Column integrated dry and wet deposition as two separate outputs (dry_x and wet_x). 3D total production rates and total loss rates to chemical reactions (prod_x and loss_x). Total production rates and total loss rates to photolysis reactions (prodphoto_x and lossphoto_x). Units are kg m^{-2} s^{-1} and kg m^{-3} s^{-1}, respectively for 2d and 3d variables.

Budget term	CF standard name	Output variable name
Emissions (2d)	tendency_of_atmosphere_mass_content_of_formaldehyde_due_to_emission	emihcho
Dry deposition (2d)	tendency_of_atmosphere_mass_content_of_formaldehyde_due_to_dry_deposition	dryhcho
Wet deposition (2d)	tendency_of_atmosphere_mass_content_of_formaldehyde_due_to_wet_deposition	wethcho

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Chemical production (3d)	tendency_of_atmosphere_mass_content_of_formaldehyde_due_to_chemical_production	prodhcho
Chemical production due to photolysis (3d) (Only for compounds where relevant)	tendency_of_atmosphere_mass_content_of_formaldehyde_due_to_chemical_production_by_photolysis	prodphotohcho
Chemical destruction (3d)	tendency_of_atmosphere_mass_content_of_formaldehyde_due_to_chemical_destruction	losshcho
Chemical destruction due to photolysis (3d) (Only for compounds where relevant)	tendency_of_atmosphere_mass_content_of_formaldehyde_due_to_chemical_destruction_by_photolysis	lossphotohcho

Table 3 lists the global atmospheric chemistry models confirmed for participation in VOCMIP. This selection of models will enable robust intercomparison and provide valuable insights into the variability and uncertainties in VOC processes across different models. However, additional models are encouraged to join VOCMIP.

Table 3: Models confirmed to take part in VOCMIP.

Model	Reference
CESM2 CAM-Chem	Emmons et al. (2020)
EC-Earth	Van Noije et al. (2021); Williams et al. (2022)
EMAC	Jöckel et al. (2016)
FRSGC/UCI CTM	Wild (2007)
GISS	Bauer et al. (2020); Kelley et al. (2020)
GFDL	Horowitz et al. (2020)
LMDZ-INCA	Folberth et al. (2006); Hauglustaine et al. (2004)
NorESM2-LM	Emmons et al. (2020); Seland et al. (2020)
OsloCTM3	Søvde et al. (2012)
UCICTM	Prather et al. (2017)
UKCA	Archibald et al. (2020a)

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Figure 2 displays the atmospheric burden of twenty major VOCs as simulated by two global atmospheric models (CESM2 WACCM and OsloCTM3). The results demonstrate a general consistency for several compounds, highlighting agreement between the models for some compounds. However, notable discrepancies are observed for certain VOCs, particularly acetone, where the models diverge significantly. Additionally, the figure reveals that some VOCs are entirely absent in one of the models, emphasizing the need for improved representation and standardization in VOC simulations. Moreover, the comparison of the burdens of the VOCs shows that there is need for the diagnostics we outline in Table 2 to understand the differences in process that control the species burdens.

3 Observational data

To better constrain the budget for VOCs, and in particular HCHO, comparison between models and observations will be performed. Satellite retrievals of VOCs will be combined with in situ surface and aircraft measurements.

3.1 Satellite data

Satellite retrievals for ten main VOCs are available, see Table 4 and Figure 2. Except for methyl hydroperoxide (MHP) and partly ethane (where only limited retrievals are available) several of the most important VOCs are covered by satellite retrievals (Figure 2). Figure 3 shows seasonal and geographical distributions of methanol column retrieved from the two satellites IASI and CrIS. The satellite data show a pronounced seasonal variation and a significant land-to-ocean gradient. Methanol concentrations are highest over forested regions, primarily due to natural emissions from vegetation, with additional contributions from biomass burning. The broad agreement between IASI and CrIS satellite data of methanol is clearly evident.

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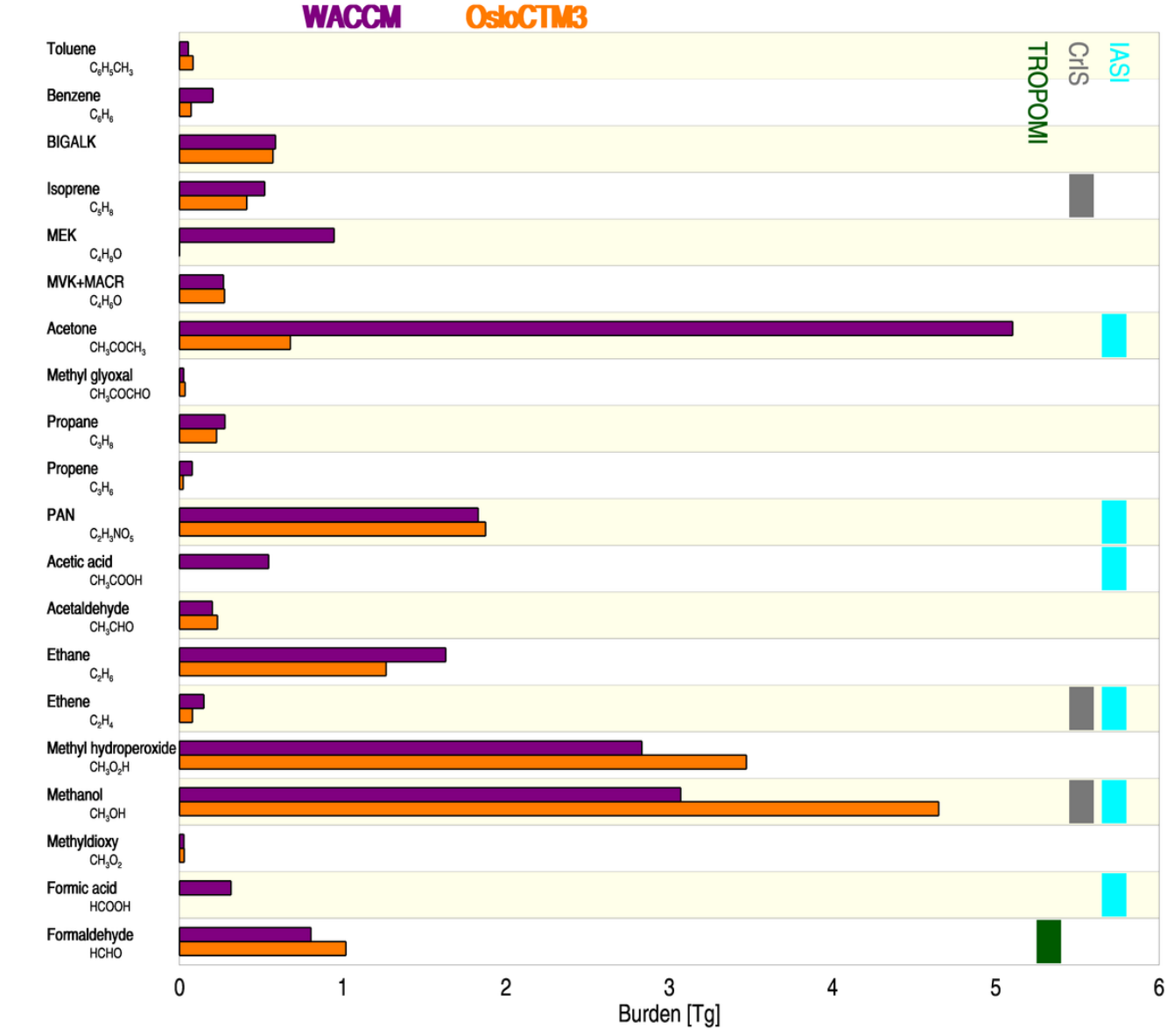

Figure 2: Global mean burden of twenty major VOCs from two global atmospheric chemistry models (OsloCTM3 and CESM2 WACCM). BIGALK includes all larger alkanes than ethane and propane. MVK is methyl vinyl ketone, MACR is methacrolein, PAN is peroxyacetyl nitrate and MEK is methyl ethyl ketone. Colours on the right-hand side indicate which satellite retrievals for IASI, CrIS and TROPOMI are available for VOCs. The simulation with WACCM6 (Gettelman et al., 2019) is set up as the CTRL simulation in Sand et al. (2023) except that slightly fewer vertical levels are used here (70 instead of 88). OsloCTM3 results are for year 2010 and taken from Skeie et al. (2025).

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Table 4: Satellite retrievals available

VOC	Chemical formula	Instrument	Reference
Acetic acid	CH_3COOH	IASI	Franco et al. (2020)
Acetone	C_3H_6O	IASI	Franco et al. (2019)
Ethane	C_2H_6	CrIS	Brewer et al. (2024)
Ethene	C_2H_4	IASI* & CrIS	Franco et al. (2022); Wells et al. (2025)
Ethyne	C_2H_2	IASI & CrIS	Wells et al. (2025)
Formaldehyde	HCHO	TROPOMI	De Smedt et al. (2021)
Formic acid	HCOOH	IASI	Franco et al. (2018); Franco et al. (2020)
Glyoxal	CHOCHO	TROPOMI	Lerot et al. (2021)
Isoprene	C_5H_8	CrIS	Wells et al. (2020); Wells et al. (2022)
Methanol	CH_3OH	IASI & CrIS	Wells et al. (2025); Franco et al. (2018)
PAN	$CH_3COO_2NO_2$	IASI	Franco et al. (2018); Zhai et al. (2024)

*limited to retrievals in biomass burning plumes and over major anthropogenic point sources.

3.2 In situ surface and aircraft data

The EBAS database (https://ebas-data.nilu.no/Default.aspx) provides access to in situ data from stations world-wide for a large number of VOCs including all but a few (MHP, CH_3O_2, PAN, MVK and BIGALK, though some of these, particularly BIGALK, may be covered or partially covered by or within categories of observations) of the compounds shown in Figure 2. The database includes contributions from networks like EMEP and ACTRIS, (Laj et al., 2024) as well as data part of intensive campaigns conducted within various projects. Some of these measurements are performed offline with DNPH (2,4-dinitrophenylhydrazine) sampling and HPLC (High-performance liquid chromatography) analysis covering aldehydes and ketones. In general, NMHC are measured with gas chromatography techniques.

In addition to surface data from measuring stations and satellite data for total column information, flight campaign data can provide granular data on the VOC composition with height. The measuring data from TOGA and PANTHER instruments includes measurements of several of the VOCs in Figure 2 except ethene, ethane, propene, methyl hydroperoxide, methyl glyoxal, methyldioxy, formic acid, acetic acid and BIGALK. The Korea–United States Air Quality (KORUS-AQ) field study was conducted during May–June 2016 (Crawford et al., 2021). Atmospheric Tomography (ATom) Mission conducted four global circuits from 2016 to 2018 (Thompson et al., 2022).

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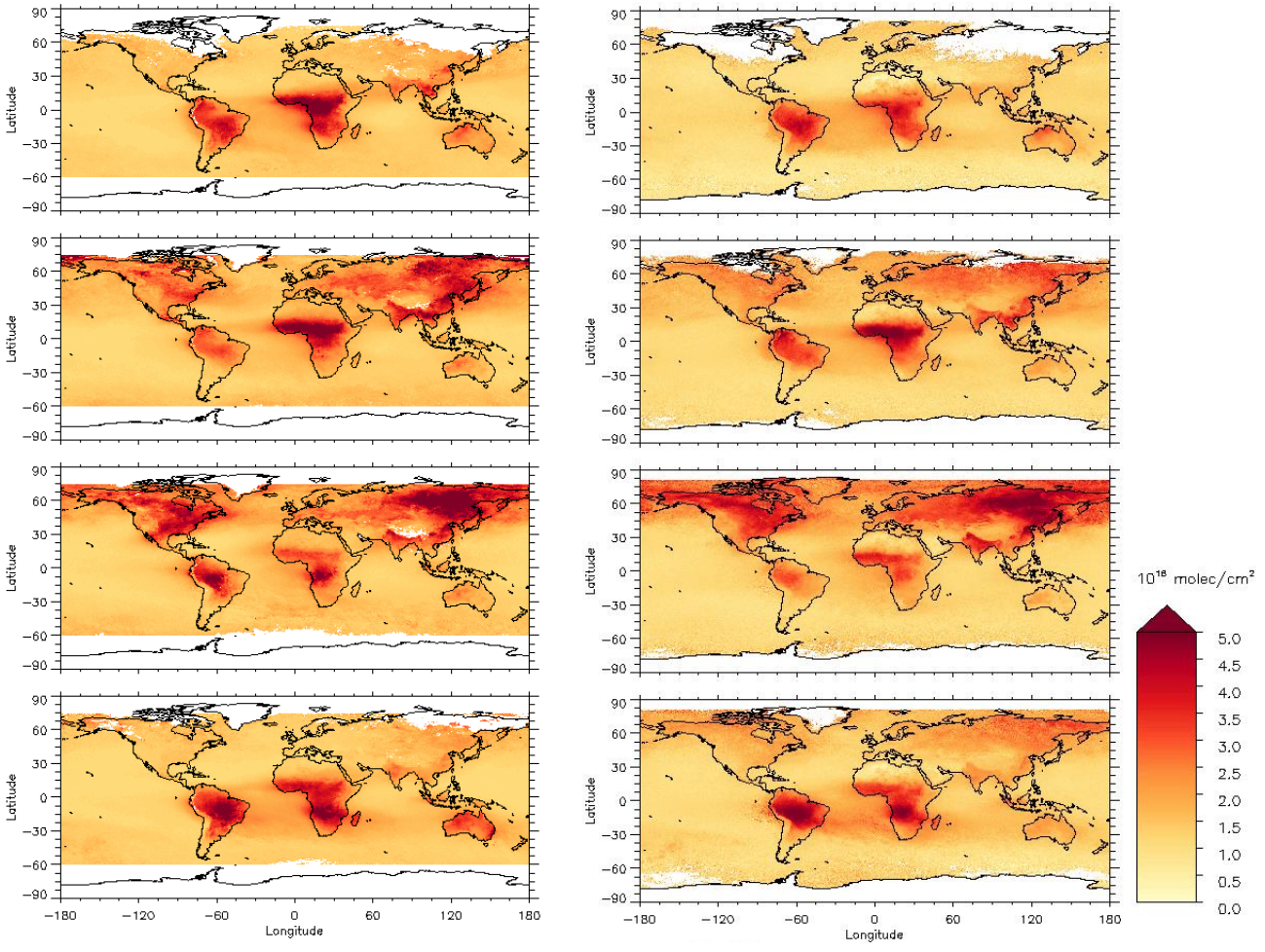

Figure 3: Satellite retrievals by CrIS (left panel) (Wells et al., 2025) and IASI (right panel) (Franco et al., 2018) of methanol column for January, February and March (top row), April, May and June (second row), July, August and September (third row), October, November and December (fourth row) for the year 2019.

4 Summary

Given the significant role of VOCs on ozone formation (Stevenson et al., 2013; Monks et al., 2015), methane lifetime (Thornhill et al., 2021), atmospheric hydrogen formation (Ehhalt and Rohrer, 2009), secondary organic aerosol formation (Kroll and Seinfeld, 2008), their accurate representation in global atmospheric chemistry models is crucial. As part of VOCMIP, satellite retrievals and in situ measurements of key VOCs will be employed to evaluate the performance of a variety of global atmospheric chemistry models. Eleven modelling groups have committed to VOCMIP, and additional modelling groups are encouraged to participate.

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Code and data availability

OsloCTM3 and WACMM data for Figure 2 are available at https://doi.org/10.5281/zenodo.15827664. The CrIS ROCRv2 VOC retrievals used in this work are available at https://doi.org/10.13020/9r8x-pp66 (Wells et al., 2025). The OsloCTM3 version used here is available at https://doi.org/10.5281/zenodo.15309428 (Sandstad and Falk, 2025). WACCM6 code is available as part of the CESM2 release via github. Instructions are at this site (http://www.cesm.ucar.edu/models/cesm2/release_download.html).

Author contributions

GM initiated the study. RBS and M Sand made Figure 1. LC, BF, DBM, and KCW provided methanol satellite data for Figure 3. All authors made input to the MIP design and writing of the manuscript.

Competing interests

At least one of the (co-)authors is a member of the editorial board of *Geoscientific Model Development*. The authors have no other competing interests to declare.

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