

Guidance on the use of AEDT Gridded Aircraft Emissions in Atmospheric Models

Version 2.0

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Document Purpose

This document describes how to interpret and implement the gridded aircraft emission fields from AEDT (Aviation Environmental Design Tool) for use in atmospheric chemistry and climate models. Revised versions of this document will be released as needed.

Primary Contacts

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Vertical and Horizontal Gridding

There are four types of altitude referred to in this guidance document:

1. Nominal: altitudes corresponding to the vertical grid index multiplied by the nominal vertical grid resolution.
2. True: altitudes above mean sea level.
3. Pressure: corresponds to the International Standard Atmosphere (ISA).

4. AGL: above ground level.

AEDT emissions are gridded onto a regular polar 3-D array: 1° latitude ($J=0:179$) by 1° longitude ($I=0:359$) by 0.5 kft (nominal) ($K=0:128$). Emissions above 45 kft (nominal) (i.e. $K>90$) are erroneous and should be discarded. The horizontal coordinates are depicted in Fig. 1. There are no emissions for $J<31$. Altitudes are in increments of 0.5 kft (nominal) starting at 0.0 kft (nominal).

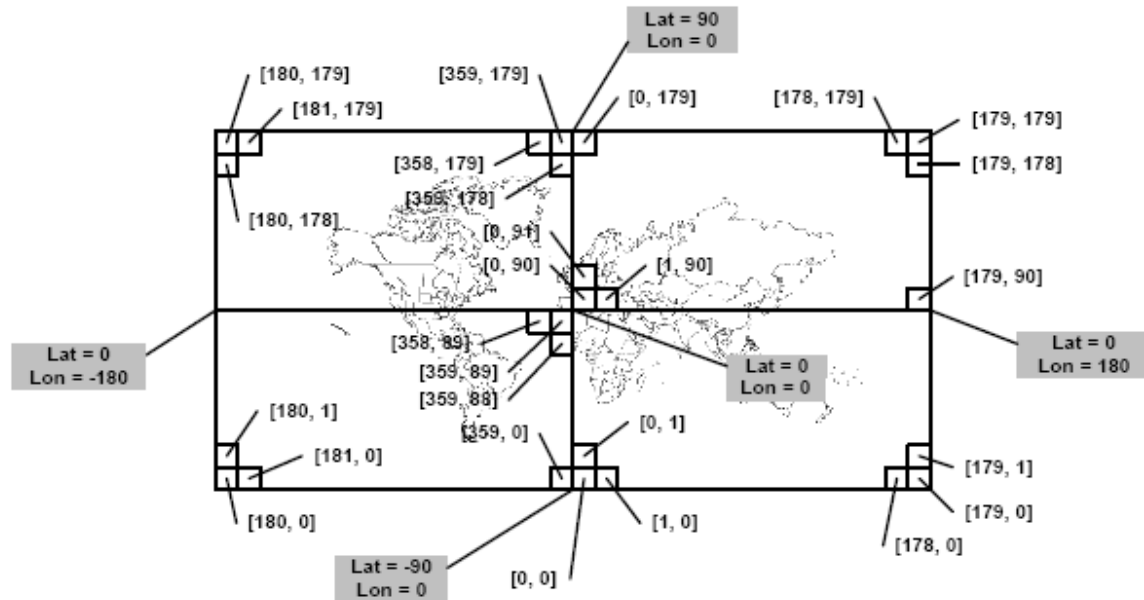


Figure 1: Schematic of horizontal grid with indices $[I,J]$.

Depending on the altitude index K , altitudes are treated differently in AEDT. All data below 10 kft (nominal) correspond to true altitudes. Above 10 kft (nominal), altitudes are pressure altitudes defined relative to the ISA shown in Table 1.

In some studies it is necessary to distinguish between impacts of landing and takeoff (LTO) emissions and non-LTO emissions. LTO operations are defined as those below 3 kft AGL. LTO emissions are therefore deposited at different values of the altitude index K depending on the corresponding surface elevation.

It is suggested that modelers:

1. Discard all emissions for $K>90$.
2. For $K>20$, treat altitudes as pressure altitudes mapping nominal altitudes to pressures given in Table 1.
3. For emissions including and below $K=20$, estimate the terrain elevation at each grid column as Z ft. (A database of terrain elevations used in AEDT is available on request.) Then deposit emissions at model levels corresponding to $(500 \times K - Z)$ ft (true). As this would require processing of emissions with knowledge of meteorological fields, a pre-processing approximation is instead to deposit emissions including and below $K=20$ at

model levels corresponding to $(500 \times \mathbf{K} - \mathbf{Z})$ ft (pressure). Note that the discontinuity in this suggestion corresponds to a discontinuity in how AEDT models flights.

Modelers may choose not to implement step 3 above and not make an altitude correction for emissions below 10 kft (nominal). The primary effect of this will be to have artificially elevated LTO emissions in locations with significant elevation.

Table 1. Pressure equivalents (hPa) for each grid cell boundary. Gridded level $\mathbf{K}=0$ is the layer 0.0-0.5 kft (nominal), i.e. 1013.25-995.07 hPa.

kft	hPa	11.5	657.20	23.5	401.28	35.5	232.80	47.5	130.78
0.0	1013.25	12.0	644.40	24.0	392.71	36.0	227.29	48.0	127.67
0.5	995.07	12.5	631.81	24.5	384.28	36.5	221.89	48.5	124.64
1.0	977.16	13.0	619.42	25.0	376.00	37.0	216.62	49.0	121.68
1.5	959.51	13.5	607.23	25.5	367.87	37.5	211.48	49.5	118.79
2.0	942.12	14.0	595.23	26.0	359.88	38.0	206.46	50.0	115.97
2.5	924.99	14.5	583.43	26.5	352.04	38.5	201.56	50.5	113.22
3.0	908.11	15.0	571.82	27.0	344.33	39.0	196.77	51.0	110.53
3.5	891.48	15.5	560.39	27.5	336.76	39.5	192.10	51.5	107.90
4.0	875.10	16.0	549.15	28.0	329.32	40.0	187.53	52.0	105.34
4.5	858.96	16.5	538.09	28.5	322.02	40.5	183.08	52.5	102.84
5.0	843.07	17.0	527.21	29.0	314.85	41.0	178.73	53.0	100.40
5.5	827.41	17.5	516.52	29.5	307.80	41.5	174.49	53.5	98.02
6.0	811.99	18.0	505.99	30.0	300.89	42.0	170.35	54.0	95.68
6.5	796.81	18.5	495.65	30.5	294.10	42.5	166.30	54.5	93.42
7.0	781.85	19.0	485.47	31.0	287.44	43.0	162.35	55.0	91.20
7.5	767.12	19.5	475.47	31.5	280.90	43.5	158.50	55.5	89.03
8.0	752.62	20.0	465.63	32.0	274.48	44.0	154.73	56.0	86.92
8.5	738.34	20.5	455.96	32.5	268.18	44.5	151.06	56.5	84.86
9.0	724.28	21.0	446.45	33.0	262.00	45.0	147.47	57.0	82.84
9.5	710.44	21.5	437.10	33.5	255.94	45.5	143.97	57.5	80.87
10.0	696.81	22.0	427.91	34.0	249.99	46.0	140.55	58.0	78.95
10.5	683.40	22.5	418.88	34.5	244.15	46.5	137.22	58.5	77.08
11.0	670.19	23.0	410.00	35.0	238.42	47.0	133.96	59.0	75.25

Files Names

The gridded data in ASCII format consists of files named as:

M_D_2006_H.txt

where **M** = month = 1:12, **D** = day-of-month = 1:31 (for months with 31 days), **H** = UTC hour = 0:23. There are a total of 8760 files and about 263 GB.

File Contents

The first line in each file is a header. Each subsequent line consists of the following ASCII data:

M, D, H, J, I, K, X1, X2, FUEL, CO, HC, NOX, PMNV, X3, PMFO, X4, X5, X6.

The first six variables (**M, D, H, J, I, K**) are integers as defined above. The remaining variables describe the emissions data, are floating point numbers, and are defined as follows:

X1	Discard - not used
X2	Discard - not used
FUEL	kg of fuel burned in grid box over the hour
CO	g of CO emitted in grid box over the hour
HC	g of total hydrocarbons emitted over the hour as CH ₄ equivalent

NOX	g of NO+NO ₂ +HONO emitted over the hour as NO ₂ equivalent
PMNV	g of BC aerosol emissions only valid for LTO emissions
X3	Discard - not used
PMFO:	g of OC aerosol emissions only valid for LTO emissions
X4	Discard - not used
X5	Discard - not used
X6	Discard - not used

As noted above, several variables should be discarded. The fields PMNV and PMFO are valid approximations of BC and OC emissions, respectively, only for LTO emissions (i.e. emissions below 3000 ft AGL). Note that for some records the fuel burn values are integers and care should be taken to ensure that model file reading routines correctly read data.

Derived Emissions

This section describes how to calculate emissions not included in AEDT, or where raw AEDT emissions should be discarded (i.e. fields **X1-X5**). AEDT fields and variables defined in this document are in bold.

CO₂ emissions as g of CO₂ = 3159 × **FUEL**. The uncertainty range for this number is 3148 to 3173 based on the C:H ratios for JP-8 fuel as inferred from the Defense Energy Support Center/Petroleum Quality Information System [*Hileman et al.*, 2010].

H₂O emissions as g of H₂O = 1231 × **FUEL**. The range is 1197-1258 [*Hileman et al.*, 2010].

NO_x emissions are given on an NO₂ mass basis. Recommended partitioning at cruise at the engine exit plane by mole fraction is: 90% NO, 9% NO₂, 1% HONO for non-LTO emissions, or 76% NO, 23% NO₂, 1% HONO for LTO emissions.

CO emissions as CO in g = **CO**.

HC emissions are in CH₄ equivalent, which is converted to total organic gases (TOG) as TOG = **HC** × 1.16 [*FAA/EPA*, 2009]. Speciation of the TOG mass is given in Appendix A. Inclusion of the different TOG species depends on the chemistry scheme being used.

BC aerosol emissions below 3000 ft AGL in g = **PMNV**. A number EI of 2×10¹⁴ [0.1×10¹⁴-6×10¹⁴] particles/kg-fuel can be assumed [*Lukachko et al.*, 2010]. Above 3000 ft AGL, BC emissions in g = **FUELBURN** × 0.03 [0.01-0.07], and a number EI of 4×10¹⁴ [1×10¹⁴-60×10¹⁴] particles/kg can be assumed [*Lukachko et al.*, 2010]. In both cases a geometric standard deviation of 1.6 [1.5-1.8] can be assumed. Appendix B provides suggestions for calculating aerosol size parameters.

OC aerosol emissions below 3000 ft AGL in g = **PMFO**. For emissions above 3000 ft AGL, organic carbon emissions in g = **FUELBURN** × 0.03 [0.01-0.07].

SO₂ and S^{VI} emissions are scaled from **FUELBURN** assuming a fuel sulfur concentration **FSC** = 600 [400-800] in mg/kg-fuel [Hileman *et al.*, 2010]. For low sulfur fuels, **FSC** = 15. A mole fraction **E** = 2 [0.5-6] in % of the fuel sulfur is emitted as S^{VI}, with the remaining (100-**E**) % being emitted as SO₂. Therefore emissions of SO₂ in g = $(\mathbf{FSC}/1000) \times [(100-\mathbf{E})/100] \times \mathbf{FUELBURN} \times (64/32)$, where it should be recalled that **FUELBURN** is in kg. Emissions of S^{VI} as SO₄ in g = $(\mathbf{FSC}/1000) \times (\mathbf{E}/100) \times \mathbf{FUELBURN} \times (96/32)$.

The emission species for S^{VI} is at the discretion of the modeler. Guidelines are to emit S^{VI} as:

- SO₃ if the model explicitly treats the aircraft exhaust plume from the engine exit plane, i.e. emissions of S^{VI} as SO₃ in g = $(\mathbf{FSC}/1000) \times (\mathbf{E}/100) \times \mathbf{FUELBURN} \times (80/32)$.
- H₂SO₄(g) if the model treats the aircraft exhaust plume from a point downstream of the engine exit plane, i.e. emissions of S^{VI} as H₂SO₄(g) in g = $(\mathbf{FSC}/1000) \times (\mathbf{E}/100) \times \mathbf{FUELBURN} \times (98/32)$.
- Sulfate aerosol if the model treats emissions at the grid scale, i.e. emissions of S^{VI} as SO₄ in g = $(\mathbf{FSC}/1000) \times (\mathbf{E}/100) \times \mathbf{FUELBURN} \times (96/32)$.

Below 3000 ft AGL, a number EI for sulfates plus organic carbon of 1×10^{16} [0.2×10^{16} - 2×10^{16}] particles/kg-fuel can be assumed with a geometric standard deviation of 1.5 [1.4-1.6]. Above 3000 ft AGL, a number EI for sulfates plus organic carbon of 2×10^{16} [1×10^{16} - 5×10^{16}] particles/kg-fuel can be assumed with a geometric standard deviation of 1.5 [1.4-1.6]. Based on Lukachko *et al.* [2010]. Appendix B provides practical suggestions for calculating aerosol parameters.

Checksums for AEDT emissions are given in Table 2.

Table 2. Checksums for AEDT data set of Year 2006 emissions. In total there are 1,157,687,013 hourly records.

Variable		#	Min	Max	Sum
M	Month	1	1	12	
D	Day	2	1	31	
H	Hour	3	0	23	
J	Latitude index	4	31	179	
I	Longitude index	5	0	359	
K	Altitude index	6	0	128	
FUEL	Fuel burn (kg)	9	0.00E+00	1.79E+05	1.88104E+11
CO	CO (g)	10	0.00E+00	2.21E+06	6.76082E+11
HC	HC (g)	11	0.00E+00	4.16E+05	9.75864E+10
NOX	NO _x as NO ₂ (g)	12	0.00E+00	5.05E+06	2.66710E+12
PMNV	BC aerosol	13	0.00E+00	6.21E+03	6.80500E+09
PMFO	OC aerosol	15	0.00E+00	1.28E+05	1.34824E+11

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Appendix A (Speciation of Total Organic Gases)

Also available at: <http://www.epa.gov/oms/regs/nonroad/aviation/420r09903.xls>

Species	Mass Fraction
Ethylene	0.15458986
Acetylene	0.039385952
Ethane	0.005214505
Propylene	0.045336437
Propane	0.000780871
Isobutene/1-Butene	0.017538274
1,3-Butadiene	0.016869627
cis-2-Butene	0.002104593
3-Methyl-1-butene	0.001122751
1-Pentene	0.007760686
2-Methyl-1-butene	0.001395718
n-Pentane	0.00198433
trans-2-Pentene	0.003593968
cis-2-Pentene	0.002757017
2-Methyl-2-butene	0.001846216
4-Methyl-1-pentene	0.000686543
2-Methylpentane	0.004084956
2-Methyl-1-pentene	0.000342498
1-Hexene	0.00736025
trans-2-Hexene	0.000296913
Benzene	0.01681482
1-Heptene	0.004384568
n-Heptane	0.000638894
Toluene	0.006421156
1-Octene	0.002757017
n-Octane	0.000624801
Ethylbenzene	0.001742866
m-Xylene/p-Xylene	0.002821783
Styrene	0.003094253
o-Xylene	0.001659872
1-Nonene	0.002455358
n-Nonane	0.000623583
Isopropylbenzene	3.16893E-05
n-Propylbenzene	0.000532688
m-Ethyltoluene	0.001541363
p-Ethyltoluene	0.000641639
1,3,5-Trimethylbenzene	0.000540657
o-Ethyltoluene	0.000654377
1,2,4-Trimethylbenzene	0.003501888
1-Decene	0.001846216
n-Decane	0.003201988

1,2,3-Trimethylbenzene	0.001062139
n-Undecane	0.004441511
n-Dodecane	0.004615541
n-Tridecane	0.005354028
C14-alkane	0.00186031
C15-alkane	0.00177053
n-tetradecane	0.00416355
C16-alkane	0.001459826
n-pentadecane	0.001726267
n-hexadecane	0.000486609
C18-alkane	1.76775E-05
n-heptadecane	8.84283E-05
phenol	0.007261785
naphthalene	0.00541181
2-methyl naphthalene	0.002061886
1-methyl naphthalene	0.002466177
dimethylnaphthalenes	0.000898492
C4-Benzene + C3-aroald	0.006564325
C5-Benzene+C4-aroald	0.003241136
Methanol	0.018051895
Formaldehyde (FAD)	0.123081099
Acetaldehyde (AAD)	0.042718224
Acetone	0.003693477
Propionaldehyde	0.007265856
Crotonaldehyde	0.010327611
Butyraldehyde	0.001185413
Benzaldehyde	0.004695067
Isovaleraldehyde	0.000324866
Valeraldehyde	0.002451834
o-Tolualdehyde	0.002297695
m-Tolualdehyde	0.002777561
p-Tolualdehyde	0.000481828
Methacrolein	0.004290087
Glyoxal	0.018164641
Methylglyoxal	0.015032806
acrolein	0.024493139
Total	0.707868569
<i>C-10 paraffins*</i>	<i>0.14608</i>
<i>C-10 olefins*</i>	<i>0.05843</i>
<i>decanal*</i>	<i>0.05843</i>
<i>dodecenal*</i>	<i>0.02922</i>
Total inc. unidentified*	1.0000

* 29% of unidentified mass was assigned based on judgment [FAA/EPA, 2009].

Appendix B (Guidance on Calculating PM Size Distribution Parameters)

Steven Barrett, Stephen Lukachko and Ian Waitz, MIT

Lukachko et al. (2010) characterizes the mass EI (denoted M in this appendix), number EI (N), geometric mean diameter (D) and geometric standard deviation (σ) of aircraft primary BC, OC and sulfate emissions in terms of nominal values and ranges. Note, however, that these are not independent parameters and direct use of M , N and D as independent variables in models would not generally lead to consistent results. In this appendix we provide an approach to calculating consistent sets of aerosol parameters assuming that non-volatile PM is log-normally distributed, and that volatile PM is log-normally distributed. We assume non-volatile PM is black carbon (BC), while volatile PM in this context is sulfate as H_2SO_4 plus organic carbon (OC).

First, assume M and N are the independent parameters with a nominal value, lower and upper bound as given in the main body of this document. Considering non-volatile PM first, Lukachko et al. (2010) describes the nominal [range] of values of the geometric standard deviation to be 1.6 [1.5-1.8]. Given the uncertainty in N and M dominates, we suggest fixing the geometric standard deviation for non-volatile PM at $\sigma_{NV} = 1.6$.

Assuming a log-normal size distribution, it can be shown that

$$M = \frac{\pi}{6} \rho D^3 N \exp\left[\frac{9}{2}(\ln \sigma)^2\right], \quad (1)$$

where ρ is the effective density of the aerosol (Heintzenberg, 1994). For BC, $\rho_{NV} = \rho_{BC} = 1000 \text{ kg/m}^3$ (Onasch et al., 2009) was assumed for the effective density. Thus the geometric mean diameter for the non-volatiles can be calculated as

$$D_{NV} = \left[\frac{M_{NV}}{1.415 \rho_{NV} N_{NV}} \right]^{1/3}. \quad (2)$$

Note that here only SI units are used. For example, mass EIs (conventionally in g/kg-fuel) need to be divided by 10^3 to convert to SI units before use in Eq. (2).

For a log-normal distribution, the surface area EI (i.e. m^3 of aerosol surface area per kg of fuel burnt) is given by

$$S = \pi D^2 N \exp[2(\ln \sigma)^2], \quad (3)$$

which for non-volatiles becomes

$$S_{NV} = 4.887 D_{NV}^2 N_{NV} \quad (4)$$

if spherical particles are assumed, which may be inappropriate for non-volatile PM (Onasch et al., 2009). We note that assuming a single log-normal non-volatile distribution is a simplification.

Considering now the volatile PM distribution, the number EI is given in the main body of this document and Lukachko et al. (2010) as a total for all volatile PM. Recent measurements

(Onasch et al., 2009; Timko et al., 2010) suggest that volatile PM is a single distribution of internally mixed OC and H₂SO₄.

Assuming both sulfate and OC particles form a single distribution of internally mixed OC and H₂SO₄, it can be shown that the geometric mean diameter for the volatile distribution is

$$D_V = \left[\frac{M_{OC} / \rho_{H_2SO_4} + M_{H_2SO_4} / \rho_{OC}}{1.097 N_V} \right]^{1/3}, \quad (5)$$

where it has been assumed that for the volatile aerosol distribution $\sigma_V = 1.5$. It can be assumed that $\rho_{OC} = 900 \text{ kg/m}^3$ (Onasch et al., 2009) and $\rho_{H_2SO_4} = 1840 \text{ kg/m}^3$. Note that $M_{H_2SO_4}$ should be calculated given an assumed fuel sulfur content and S^{IV} to S^{VI} conversion fraction for consistency. The surface area EI is

$$S_V = 4.364 D_V^2 N_V. \quad (6)$$

We note that a significant fraction of volatile material is a coating on non-volatile PM (Onasch et al., 2009). This has not been taken account of above – all volatile mass has been assigned to the nucleation mode. As a sensitivity modelers may apportion 50% of volatile mass to the internally mixed nucleation mode, and the balance as a soot coating. It is thought that at low thrust settings the nucleation mode dominates, at high thrust settings the condensation mode dominates, while at intermediate thrust settings (including cruise) both modes are of the same order. We also note that the volatile distribution is likely representative of an aged plume and modelers may chose to apply different size or number constraints in cases where plume evolution is explicitly modeled. For example, constraining the volatile size distribution of a young plume by assuming a geometric mean diameter of 5 nm would be an appropriate sensitivity.

Examples for Cruise Emissions

Using the range for the non-volatile mass EI of $M_{NV} = 0.03$ [0.01 – 0.07] g/kg – fuel and number EI of $N_{NV} = 4 \times 10^{14}$ [$1 \times 10^{14} - 60 \times 10^{14}$] particles/kg – fuel we find the following estimates of the geometric mean diameter:

D_{NV} (nm)	Low N_{NV}	Nominal N_{NV}	High N_{NV}
Low M_{NV}	41	26	11
Nominal M_{NV}	60	38	15
High M_{NV}	79	50	20

Lukachko et al. (2010) reported D_{NV} is typically in the range 30-60 nm.

Similarly, using the range for the organics EI of $M_{OC} = 0.03$ [0.01 – 0.07] g/kg – fuel, and assuming a fixed $M_{H_2SO_4} = 0.04$ g/kg – fuel (based on $FSC = 600$ and $E = 2$) and total volatile number EI of $N_V = 2 \times 10^{16}$ [$1 \times 10^{16} - 5 \times 10^{16}$] particles/kg – fuel we find the following estimates of the geometric mean diameter:

D_v (nm)	Low N_v	Nominal N_v	High N_v
Low M_{OC}	14	11	8
Nominal M_{OC}	17	14	10
High M_{OC}	21	17	12

Lukachko et al. (2010) reported D_v is typically in the range 1-20 nm.

For LTO emissions, users can calculate the EIs for BC and OC based on the AEDT inventory. For example, for BC emissions, gridded BC emissions can be divided by fuel burn to get the local EI. Then the same procedure noted above can be applied with the number EIs noted in the main body of this document.

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Appendix C (List of Acronyms)

ACCRI	Aviation Climate Change Research Initiative
AEDT	Aviation Environmental Design Tool
AGL	Above Ground Level
APEX	Aircraft Particle Emissions Experiment
BC, OC	Black Carbon; Organic Carbon
CMAQ	Community Multiscale Air Quality (a model)
CO, HC, CH ₄	Carbon monoxide, hydrocarbon, methane
EI, nEI	Mass emission index, number emission index.
EPA	Environmental Protection Agency
FAA	Federal Aviation Administration
FOA	First Order Approximation
FSC	Fuel Sulfur Concentration (or Content)
g	Grams
GB	Gigabyte
hPa	Hecto-pascal = 100 pascals
inc.	including
kft	kilofeet (thousands of feet)
Lat	Latitude
Lon	Longitude
LTO	Landing and Takeoff
NO, NO ₂	Nitric oxide, nitrogen dioxide
NO _x ,	Oxides of nitrogen (NO+NO ₂ by definition, but assumed to include HONO mass in reporting)
PAH	Polycyclic Aromatic Hydrocarbons
PM	Particulate Matter
PMFO	Organic PM from fuel
PMNV	Black carbon with a very small amount of metals
PMSO	Sulfur particulate matter reported as SO ₄ (note that raw AEDT inventory values of PMSO should be discarded)
SO ₂ , S, H ₂ SO ₄	Sulfur dioxide, elemental sulfur, sulfuric acid
TOG	Total organic gases
UTC	Coordinated Universal Time