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SUBJECT: Assessment of Solution-Agnostic Observational Needs for Stratospheric Composition

1. Scope:

This memo provides background information and recommendations and guidance for solution-agnostic observational needs for Stratospheric Composition.

2. Background:

NESDIS has to regularly assess the user mission needs for environmental observations. This is important in order to (1) remain cognizant with the evolution of these needs and to (2) better plan for the next-generation architecture, and in particular, the space-based architecture. To achieve this goal, these needs have to be collected from a broad community, in a solution-agnostic fashion, in order to provide a reference for multiple observing systems solutions that will be able (1) to meet these needs now and in the future, (2) to look at innovative ways to meet all needs cost-effectively, and (3) to potentially fill or reduce existing observation gaps. It is important to note that these needs are expressed from a relatively wide community of observational users, but it is important to highlight they do not constitute requirements for NOAA. An internal NOAA process exists to define observational requirements. This effort is one part of the overall NESDIS user engagement process.

Understanding stratospheric composition is important due to potential impacts on human and ecosystem health and climate. The SAT subcommittee on atmospheric composition (see List of Contributors) focused on several application areas where satellite data are a main source of observational data. A panel of expert reviewers (see List of Contributors) reviewed the needs, attributes, and their priorities, following which observational needs for these applications were briefed to the SAT. Representatives were in attendance from academia, private sector, NASA, DoD, and in NOAA, from the line offices, and the OSAAP Analysis Team (TPIO) in charge of stewarding and updating the COURL, as well as representatives from the major programs, who ultimately will be charged with developing the components of the space architecture (LEO, GEO, and SWO). All were given opportunities to provide comments and feedback on the observational needs.

It is the purpose of this memo, compiled by the SAT subcommittee on atmospheric composition and reviewed by the Government-only Core-SAT team, to document and establish the needs for stratospheric composition by assessing the users' needs from many sources. It is important to note that the information captured is in geophysical space which is consistent with the international standard established by the WMO (e.g., the OSCAR database). This means that what is captured here is the information content needed for the observations. It does not mean that the user systems will assimilate those products. This exercise captured user needs in a solution-agnostic fashion.

- 3. Facts and Findings:
 - a. Facts
- Atmospheric chemistry species were selected from a subset of chemical species that are included in state-of-the-art global atmospheric chemical transport models, such as the Real-time Air Quality Modeling System (RAQMS).
- (2) Reductions in stratospheric ozone concentration allow more damaging radiation to reach the Earth's surface, potentially harming plants and animals and impacting human health and, notably, agriculture.
- (3) The distribution of stratospheric ozone has been shown to affect tropospheric conditions, including weather, on seasonal to sub-seasonal time scales, as well as impacting large scale circulation patterns.
- (4) Continual monitoring of stratospheric ozone with good global coverage on weekly to monthly time scales will feed into improved understanding of radiative and dynamical processes and improve near-term as well as seasonal to sub-seasonal forecasts.
- (5) Maintaining vertically and spatially resolved satellite measurements of both ozone, water vapor, and aerosols is critical, as are measurements of other chemically and radiatively active species in the stratosphere.
- (6) The US Clean Air Act mandates that NOAA and NASA regularly report on the state of the stratospheric ozone layer to Congress.
- (7) Stakeholders of NOAA's stratospheric ozone monitoring include numerous Federal agencies (e.g., NOAA, NASA, EPA, USDA, etc.), the private sector (agricultural interests), and a variety of international bodies.
- b. Findings
 - (1) The SAT developed a list of solution-agnostic stratospheric composition observational needs and assembled them into several tables. The tables summarize those observational needs and were determined as part of the overall NESDIS user engagement process that consisted of deliberations with experts, established expert groups, published documentation, and

NOAA Line Office experts. The list was consolidated, reviewed, and approved by the Government-only Core-SAT committee.

4. Recommendation:

The SAT recommends that NOAA use the following solution-agnostic stratospheric composition observational needs, as shown in the tables below, as an input to the establishment of the NOAA observational requirements for stratospheric composition needs. These tables include variable names, attributes' ranges of these variables, as well as associated prioritizations. These recommendations should be considered as part of the planning and development of next-generation space architecture and product development.

Table Descriptions

Table 1. Describes the list of variables needed for the stratospheric composition applications, why they are important for the application, and whether they are already identified as an existing variable in the TPIO databases.

Table 2. Identifies geophysical variable priorities for the stratospheric composition application as reviewed by the Core-SAT using the inputs from the subcommittee for atmospheric composition as an input. The recommendations from other user needs activities (TPIO, NASA-NOAA, XORWG, etc.) were considered, and included by OSAAP/TPIO.

Table 3. Shows the variable performance ranges for the stratospheric composition application, as determined by the Core-SAT. These data are based on the input from the subcommittee for atmospheric composition as well as input from the OSAAP Analysis Team, and other sources, as mentioned previously. The data ranges, shown as triplets, are defined as "minimally useful or Threshold," "Expected [performance in the 2030-time frame]," and "Maximum Effective." The current geophysical variable performance ranges are listed as well.

Table 4. Includes stratospheric composition application attribute priorities, per variable, including horizontal and vertical resolution, temporal resolution, error standard deviation, and data latency. This table was provided by the OSAAP/TPIO Team based on "differential attribute change per unit time" in the vertical and horizontal dimensions. Current attribute weights, per geophysical variable, are listed.

Conclusions:

This is the first comprehensive catalog of observational needs for stratospheric composition that has been collected by NOAA. This observational needs list is designed to consolidate the set of needs, defined in a way that helps the design and evaluation of the next-generation space architecture, but also to serve as a reference for all those interested in these needs in the near future. As stated previously, the collection of user needs was developed and reviewed by a variety of different sources that included

representatives from the OSAAP/TPIO, the LEO and GEO programs, and representatives from the NOAA Line Offices and Centers (OAR/CSL, OAR/GML, OAR/ARL, NWS/EMC, NESDIS/STAR, OAR/CPO), NASA, DoD, and academia. The final determination of the list of user needs and attributes was assembled and confirmed by the Core-SAT. The collection of observational user needs is part of the on-going user engagement process and should be refreshed regularly in order to maintain an up-to-date list of users' observational needs.

<u>**Table 1. Stratospheric Composition Variable Needs:**</u> Table 1 is a list of the variables needed by the stratospheric composition application, the importance of these variables, and a notation about the variable status in the TPIO databases.

| Geophysical Variable | Variable Importance | TPIO Database (Existing/ New) |
|---|--|----------------------------------|
| O3 – Ozone | Key constituent of the stratosphere protecting human and ecosystem health and climate | Е |
| N2O – Nitrous Oxide | Ozone depleting substance, tracer for chemical and dynamical processes | N |
| CH4 – Methane | Tracer for chemical and dynamical processes | Е |
| CO2 – Carbon Dioxide | Tracer for chemical and dynamical processes | Е |
| CFCl3 (F11) – Trichlorofluoromethane | Ozone depleting substance | Ν |
| CF2Cl2 (F12) – Dichlorodifluoromethane | Ozone depleting substance | N |
| CH3Br – Bromomethane | Ozone depleting substance | N |
| CF3Br (H1301) – Bromotrifluoromethane | Ozone depleting substance | Ν |
| CF2ClBr (H1211) – Bromochlorodifluoromethane | Ozone depleting substance | Ν |
| HNO3 - Nitric Acid | Tracer for chemical and dynamical processes | Е |
| N2O5 – Dinitrogen Pentoxide | Tracer for chemical and dynamical processes | N |
| H2O2 – Hydrogen Peroxide | Tracer for chemical and dynamical processes | N |
| HCl – Hydrogen Chloride | Tracer for chemical and dynamical processes | N |
| ClONO2 – Chlorine Nitrate | Tracer for chemical and dynamical processes | N |
| ClO - Chlorine Monoxide | Tracer for chemical and dynamical processes | N |
| OClO – Chlorine Dioxide | Tracer for chemical and dynamical processes | N |
| HF - Hydrogen Fluoride | Tracer for chemical and dynamical processes | N |
| HNO4 – Peroxynitric Acid | Tracer for chemical and dynamical processes | N |
| HOCl – Hypochlorous Acid | Tracer for chemical and dynamical processes | N |
| NO3 – Nitrate | Tracer for chemical and dynamical processes | N |
| NO2 – Nitrogen Dioxide | Tracer for chemical and dynamical processes | Е |
| NO – Nitrogen Oxide | Tracer for chemical and dynamical processes | N |
| CH3OOH – Methyl Hydroperoxide | Tracer for chemical and dynamical processes | N |
| CO – Carbon Monoxide | Tracer for chemical and dynamical processes | Е |
| HBr – Hydrogen Bromide | Tracer for chemical and dynamical processes | N |
| BrO – Bromine | Tracer for chemical and dynamical processes | N |
| BrONO2 – Bromine Nitrate | Tracer for chemical and dynamical processes | N |
| HOBr – Hypobromous Acid | Tracer for chemical and dynamical processes | N |

| Geophysical Variable | Variable Importance | TPIO Database (Existing/ New) |
|----------------------------------|---|----------------------------------|
| BrCl – Bromine Chloride | Tracer for chemical and dynamical processes | N |
| Cl2 – Chlorine | Tracer for chemical and dynamical processes | N |
| Aerosol Optical Depth | Proxy for climate forcing by particles | Е |
| Aerosol Layer Height | Informs climate forcing by particles | Е |
| Aerosol Single Scattering Albedo | Informs climate forcing by particles | Ν |
| Aerosol Refractive Index | Informs climate forcing by particles | Е |
| Aerosol Particle Size | Informs climate forcing by particles | Е |
| Aerosol Particle Shape | Informs climate forcing by particles | N |
| Speciated Aerosol Mass | Informs climate forcing by particles | N |
| Volcanic Ash | Informs climate forcing by particles and aircraft hazard | Е |
| H2O - Water Vapor | Driver for climate forcing and tracer for chemical and dynamical processes | N |
| SO2 - Sulfur Dioxide | Informs climate forcing by particles | Е |
| SF6 - Sulphur Hexafluoride | Tracer for chemical and dynamical processes | N |
| OH - Hydroxyl Radical | Tracer for chemical and dynamical processes | N |
| HO2 - Hydroperoxy Radical | Tracer for chemical and dynamical processes | N |

Table 2. Geophysical Variable Priorities for Stratospheric Composition: This table includes the list of the geophysical information and their prioritization, based on a scale from 0 (non-important) to 1 (critically important), needed for stratospheric composition as determined by the Systems performance Assessment team (SAT). This list was consolidated using a multitude of sources and follows the variables definition and units used in the Advanced Systems Performance Evaluation tool for NOAA (ASPEN) tool.

| Geophysical Variable | Short Name | Units | Priority |
|--|------------|-------|----------|
| O3 – Ozone | O3 | ppmv | 1.0 |
| N2O – Nitrous Oxide | N2O | ppbv | 0.8 |
| CH4 – Methane | CH4 | ppbv | 0.8 |
| CO2 – Carbon Dioxide | CO2 | ppmv | 0.5 |
| CFCl3 (F11) – Trichlorofluoromethane | CFC13 | pptv | 0.5 |
| CF2Cl2 (F12) – Dichlorodifluoromethane | CF2Cl2 | pptv | 0.5 |
| CH3Br – Bromomethane | CH3Br | pptv | 0.3 |
| CF3Br (H1301) – Bromotrifluoromethane | CF3Br | pptv | 0.5 |
| CF2ClBr (H1211) – Bromochlorodifluoromethane | CF2ClBr | pptv | 0.5 |
| HNO3 - Nitric Acid | HNO3 | ppbv | 1.0 |
| N2O5 – Dinitrogen Pentoxide | N2O5 | pptv | 1.0 |
| H2O2 – Hydrogen Peroxide | H2O2 | ppbv | 1.0 |
| HCl – Hydrogen Chloride | HCl | ppbv | 1.0* |
| ClONO2 – Chlorine Nitrate | CIONO2 | ppbv | 0.8 |
| ClO - Chlorine Monoxide | ClO | pptv | 0.8 |
| OCIO – Chlorine Dioxide | OClO | pptv | 0.8 |
| HF - Hydrogen Fluoride | HF | pptv | 0.5 |
| HNO4 – Peroxynitric Acid | HNO4 | ppbv | 0.8 |
| HOCl – Hypochlorous Acid | HOCI | ppbv | 0.8 |
| NO3 – Nitrate | NO3 | ppbv | 1.0 |
| NO2 – Nitrogen Dioxide | NO2 | ppbv | 1.0 |
| NO – Nitrogen Oxide | NO | ppbv | 1.0 |
| CH3OOH – Methyl Hydroperoxide | СНЗООН | ppbv | 0.3 |
| CO – Carbon Monoxide | СО | ppmv | 0.8 |
| HBr – Hydrogen Bromide | HBr | pptv | 1.0* |
| BrO – Bromine | BrO | pptv | 0.8 |
| BrONO2 – Bromine Nitrate | BrONO2 | pptv | 0.8 |
| HOBr – Hypobromous Acid | HOBr | pptv | 0.8 |

| Geophysical Variable | Short Name | Units | Priority |
|----------------------------------|-----------------------|----------|----------|
| BrCl – Bromine Chloride | BrCl | pptv | 0.8 |
| Cl2 – Chlorine | Cl2 | pptv | 0.8 |
| Aerosol Optical Depth | AOD | unitless | 1.0 |
| Aerosol Layer Height | Aerosol Height | km | 0.8 |
| Aerosol Single Scattering Albedo | Aerosol Albedo | unitless | 0.8 |
| Aerosol Refractive Index | Aerosol Scattering | unitless | 0.5 |
| Aerosol Particle Size | Aerosol Size | microns | 0.8 |
| Aerosol Particle Shape | Aerosol Shape | unitless | 0.5 |
| Speciated Aerosol Mass | Speciated Aer Mass | ug/m3 | 1.0 |
| Volcanic Ash | Vol Ash | mg/m3 | 1.0 |
| H2O - Water Vapor | H2O | ppmv | 1.0 |
| SO2 - Sulfur Dioxide | SO2 | pptv | 1.0 |
| SF6 - Sulphur Hexafluoride | SF6 | ppmv | 0.5 |
| OH – Hydroxyl Radical | ОН | pptv | 0.8 |
| HO2 – Hydroperoxy Radical | HO2 | pptv | 0.8 |

<u>**Table 3. Stratospheric Composition Observational Need Attribute Performance Ranges:</u> List of observational needs of the current systems for stratospheric composition in NOAA. These needs are expressed in terms of ranges between minimally useful (Threshold), expected level of performance in 2030 (Expected) and the maximum effective usefulness level beyond which there is no incentive to improve performance (Maximum Effective).** These are written as [Threshold, Expected, Maximum Effective]. The attributes include the spatial coverage, the horizontal resolution, the temporal refresh, the precision, and latency. When appropriate, the vertical resolution is listed.</u>

- Geographic Coverage: The geographic region needed for observations.
- Horizontal resolution: The ground projected instantaneous field of view.
- Temporal refresh: Time between observations at a location, i.e, time to observe the geographic coverage region.
- Data Latency: Time from 'image taken' to full relay of data to a ground station.
- Vertical Resolution (when appropriate): The average vertical distance between observations in degrees of freedom.
- Precision: Error standard deviation under clear/cloudy conditions and over land/ocean.
- Accuracy: Mean absolute non-random error.
- Validity Range: The low and high values that can be observed.
- Long term stability of the measurement: Long term changes in precision (noise).
- Robustness: The number of sources needed to make the observation.
- Continuity: Period in years for which the observations are required.

| Geophysical Variable | Geophysical Variable Units | Geographic Coverage (dimensionless) | Horizontal Resolution (km) | Temporal Refresh (h) | Data Latency (h) | Vertical Resolution (dof) | Precision: Clear/ Cloudy, Land/ Ocean (%) | Accuracy (%) | Validity Range (Same Units as Variable) | Long- term Stability (%) | Robustness (unitless) | Continuity (yr) |
|---|-------------------------------|---|-------------------------------|-------------------------|---------------------|------------------------------|--|--------------------|---|--------------------------------|--------------------------|--------------------|
| O3 – Ozone | ppmv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1**, 5, 120] | [20, 5, 1] % | 0.001+[10, 5, 1] % | [0.001-15] | [5, 2, 1] %/Decade | [2, 3, 6] | 1 year |
| N2O – Nitrous Oxide | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [30, 15, 5] % | 1+[30, 15, 5] % | [1-400] | [10, 5, 1] %/Decade | [2, 3, 6] | 1 year |
| CH4 – Methane | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [50, 20, 5] % | 1+[25, 10, 5] % | [1-2500] | [25, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| CO2 – Carbon Dioxide | ppmv | Network, CONUS, Global | [200, 100, 20] | [72, 24, 12] | [36, 12, 6] | [1, 5, 120] | [40, 10, 5] % | [40, 10, 5] % | [250-2000] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| CFCl3 (F11) – Trichlorofluorometha ne | pptv | Network, CONUS, Global | [200, 100, 20] | [72, 24, 12] | [36, 12, 6] | [1, 5, 120] | [20, 10, 1] % | 1+[10, 5, 1] % | [1-300] | [10, 5, 1] %/Decade | [2, 3, 6] | 1 year |

| Geophysical Variable | Geophysical Variable Units | Geographic Coverage (dimensionless) | Horizontal Resolution (km) | Temporal Refresh (h) | Data Latency (h) | Vertical Resolution (dof) | Precision: Clear/ Cloudy, Land/ Ocean (%) | Accuracy (%) | Validity Range (Same Units as Variable) | Long- term Stability (%) | Robustness (unitless) | Continuity (yr) |
|---|-------------------------------|---|-------------------------------|-------------------------|---------------------|------------------------------|--|---------------------|---|--------------------------------|--------------------------|--------------------|
| CF2Cl2 (F12) – Dichlorodifluoromet hane | pptv | Network, CONUS, Global | [200, 100, 20] | [72, 24, 12] | [36, 12, 6] | [1, 5, 120] | [20, 10, 1] %% | 1+[10, 5, 1] % | [1-600] | [10, 5, 1] %/Decade | [2, 3, 6] | 1 year |
| CH3Br – Bromomethane | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [40, 10, 5] % | [40, 10, 5] % | [1-20] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| CF3Br (H1301) – Bromotrifluorometha ne | pptv | Network, CONUS, Global | [200, 100, 20] | [72, 24, 12] | [36, 12, 6] | [1, 5, 120] | [20, 10, 1] % | [10, 5, 1] % | [1-10] | [10, 5, 1] %/Decade | [2, 3, 6] | 1 year |
| CF2ClBr (H1211) – Bromochlorodifluoro methane | pptv | Network, CONUS, Global | [200, 100, 20] | [72, 24, 12] | [36, 12, 6] | [1, 5, 120] | [20, 10, 1] % | [10, 5, 1] % | [1-10] | [10, 5, 1] %/Decade | [2, 3, 6] | 1 year |
| HNO3 - Nitric Acid | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [40, 20, 5] % | [20, 10, 5] % | [1-30] | [20, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| N2O5 – Dinitrogen Pentoxide | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [50, 20, 5] % | 1+[25, 10, 5] % | [1-1000] | [25, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| H2O2 – Hydrogen Peroxide | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | 0.001+[40, 10, 5] % | [0.001-10] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| HCl – Hydrogen Chloride | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [20, 10, 1] % | 0.001+[10, 5, 1] % | [0.001-10] | [10, 5, 1] %/Decade | [2, 3, 6] | 1 year |
| ClONO2 – Chlorine Nitrate | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [30, 20, 5] % | 0.001+[15, 10, 5] % | [0.001-10] | [15, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| ClO - Chlorine Monoxide | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 40, 10] % | 0.1+[40, 20, 10] % | [0.1-10] | [40, 20, 10] %/Decade | [2, 3, 6] | 1 year |
| OClO – Chlorine Dioxide | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | [40, 10, 5] % | [0.1-5] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| HF - Hydrogen Fluoride | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [40, 20, 5] % | 1+[20, 10, 5] % | [1-2500] | [20, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| HNO4 – Peroxynitric Acid | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | 0.1+[40, 10, 5] % | [0.1-50] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| HOCl – Hypochlorous Acid | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | 0.001+[40, 10, 5] % | [0.001-50] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |

| Geophysical Variable | Geophysical Variable Units | Geographic Coverage (dimensionless) | Horizontal Resolution (km) | Temporal Refresh (h) | Data Latency (h) | Vertical Resolution (dof) | Precision: Clear/ Cloudy, Land/ Ocean (%) | Accuracy (%) | Validity Range (Same Units as Variable) | Long- term Stability (%) | Robustness (unitless) | Continuity (yr) |
|-------------------------------------|-------------------------------|---|-------------------------------|-------------------------|---------------------|------------------------------|--|----------------------|---|--------------------------------|--------------------------|--------------------|
| NO3 – Nitrate | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | 0.001+[40, 10, 5] | [0.001-50] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| NO2 – Nitrogen Dioxide | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | 1+[40, 10, 5] % | [1-100] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| NO – Nitrogen Oxide | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [20, 10, 1] % | 0.001+[10, 5, 1] % | [0.001-100] | [10, 5, 1] %/Decade | [2, 3, 6] | 1 year |
| CH3OOH – Methyl Hydroperoxide | ppbv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | 0.001+[40, 10, 5] % | [0.001-10] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| CO – Carbon Monoxide | ppmv | Network, CONUS, Global | [200, 100, 20] | [72, 24, 12] | [36, 12, 6] | [1, 5, 120] | [80, 40, 10] % | 0.001+[40, 20, 10] % | [0.001-10] | [40, 20, 10] %/Decade | [2, 3, 6] | 1 year |
| HBr – Hydrogen Bromide | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | 1+[40, 10, 5] % | [1-50] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| BrO – Bromine | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [60, 20, 10] % | [30, 20, 10] % | [1-50] | [30, 20, 10] %/Decade | [2, 3, 6] | 1 year |
| BrONO2 – Bromine Nitrate | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | [40, 10, 5] % | [1-50] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| HOBr – Hypobromous Acid | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | [40, 10, 5] % | [1-50] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| BrCl – Bromine Chloride | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | 0.01+[40, 10, 5] % | [0.01-10] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| Cl2 – Chlorine | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [1, 5, 120] | [80, 20, 5] % | 1.0+[40, 10, 5] % | [1.0-20,000] | [40, 10, 5] %/Decade | [2, 3, 6] | 1 year |
| Aerosol Optical Depth | unitless | Network, CONUS, Global | [50, 5, 1] | [1440, 60, 5] min | [180, 30, 5] min | [1, 5, 120] | [20, 10, 1] % | 0.001+[10, 5, 1] % | 0 - 50 | [10, 5, 1] %/Decade | [2, 3, 6] | 1 year |
| Aerosol Layer Height | km | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] | [5, 60, 120] | [20, 10, 1] % | 0.1+[10, 5, 1] % | 0 - 60 | NA | [2, 3, 6] | 1 year |
| Aerosol Single Scattering Albedo | unitless | Network, CONUS, Global | [10, 2, 0.1] | [24, 12, 1] | [3, 1, 0.5] | [1,5,120] | [80, 40, 5] % | 0.01+[40, 20, 5] | 0 - 1 | [40, 20, 5] %/Decade | [2, 3, 6] | 1 year |
| Aerosol Refractive | unitless | Network, CONUS, Global | [10, 2, 0.1] | [24, 12, 1] | [3, 1, 0.5] | [1,5,120] | NA | NA | 0.0001-2 | NA | [2, 3, 6] | 1 year |

| Geophysical Variable | Geophysical Variable Units | Geographic Coverage (dimensionless) | Horizontal Resolution (km) | Temporal Refresh (h) | Data Latency (h) | Vertical Resolution (dof) | Precision: Clear/ Cloudy, Land/ Ocean (%) | Accuracy (%) | Validity Range (Same Units as Variable) | Long- term Stability (%) | Robustness (unitless) | Continuity (yr) |
|-------------------------------|-------------------------------|---|-------------------------------|-------------------------|---------------------|------------------------------|--|---------------------|---|--------------------------------|--------------------------|--------------------|
| Index | | | | | | | | | | | | |
| Aerosol Particle Size | microns | Network, CONUS, Global | [10, 2, 0.1] | [24, 12, 1] | [3, 1, 0.5] | [1,5,120] | [80, 40, 5] % | 0.1+[40, 20, 5] % | 0 - 100 | [40, 20, 5] %/Decade | [2, 3, 6] | 1 year |
| Aerosol Particle Shape | unitless | Network, CONUS, Global | [10, 2, 0.1] | [24, 12, 1] | [3, 1, 0.5] | [1,5,120] | NA | NA | NA | NA | [2, 3, 6] | 1 year |
| Speciated Aerosol Mass | ug/m3 | Network, CONUS, Global | [10, 2, 0.1] | [1440, 60, 5] min | [180, 30, 5] min | [1,5,120] | [80, 40, 5] % | 2+[40, 20, 5] % | 0-1000 | [40, 20, 5] %/Decade | [2, 3, 6] | 1 year |
| Volcanic Ash | mg/m3 | Network, CONUS, Global | [4, 2, 1] | [720, 10, 1] min | [60, 10, 1 min] | [1,5,120] | [80, 40, 5] % | 0.01+[40, 20, 5] % | 0.01-1000 | [40, 20, 5] %/Decade | [2, 3, 6] | 1 year |
| H2O - Water Vapor | ppmv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] min | [1, 5, 60] | [20, 10, 5]% | [20, 10, 5]% | 1-20 | [5, 2, 1] %/Decade | [2, 3, 6] | 1 year |
| SO2 - Sulfur Dioxide | pptv | Network, CONUS, Global | [4, 2, 1] | [720, 10, 1] min | [60, 10, 1] min | [1,5,120] | 40, 20, 5] % | 0.001+[40, 10, 5] % | [1- 5000] | [5, 2, 1] %/Decade | [2, 3, 6] | 1 year |
| SF6 - Sulphur hexafluoride | pptv | Network, CONUS, Global | [200, 100, 20] | [72, 24, 12] | [36, 12, 6] min | [1, 5, 120] | [20, 10, 1] % | [10, 5, 1] % | [0-10] | [10, 5, 1] %/Decade | [2, 3, 6] | 1 year |
| OH – Hydroxyl Radical | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] | [3, 1, 0.5] min | [1, 5, 120] | [80, 40, 10] % | 0.01+[40, 20, 10] % | [0.01-10] | [40, 20, 10] %/Decade | [2, 3, 6] | 1 year |
| HO2 – Hydroperoxy radical | pptv | Network, CONUS, Global | [50, 5, 1] | [24, 12, 1] min | [3, 1, 0.5] min | [1, 5, 120] | [80, 40, 10] % | 0.01+[40, 20, 10] % | [0.01-10] | [40, 20, 10] %/Decade | [2, 3, 6] | 1 year |

* Surface to 60 km

** Must include surface

Table 4. Stratospheric Composition Observational Need Attribute Priority: List of the stratospheric composition variables as prioritized in Table 1. This table contains the relative importance of the attributes for each of the variables. This provides engineers and designers of sensors and constellations the ability to assess where emphasis should be put when performing trade studies. For each row (variable), the weights between 0 (no importance) and 1 (highest importance) is assigned to the individual attributes described in the columns. NA indicates not applicable.

| Geophysical Variable | Images | Geographic Coverage | Horizontal Resolution | Temporal Refresh | Data Latency | Vertical Resolution | Precision: Clear/ Cloudy, Land/ Ocean | Accuracy | Validity Range | Long- term Stability | Robustness | Continuity |
|---|--------|------------------------|--------------------------|---------------------|-----------------|------------------------|--|----------|----------------|-------------------------|------------|------------|
| O3 – Ozone | 1 | 1 | 1 | 1 | 0.8 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| N2O – Nitrous Oxide | 0.75 | 1 | 0.5 | 0.5 | 0.5 | 0.75 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| CH4 – Methane | 0.75 | 1 | 0.5 | 0.5 | 0.5 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| CO2 – Carbon Dioxide | 0.5 | 1 | 0.5 | 0.5 | 0.5 | 0.5 | 1 | 1 | 1 | 1 | 1 | 1 |
| CFCl3 (F11) – Trichlorofluoromethan e | 0.5 | 1 | 0.5 | 0.5 | 0.5 | 0.5 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| CF2Cl2 (F12) – Dichlorodifluorometha ne | 0.5 | 1 | 0.5 | 0.5 | 0.5 | 0.5 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| CH3Br – Bromomethane | 0.5 | 1 | 0.5 | 0.5 | 0.5 | 0.5 | 1 | 1 | 1 | 1 | 1 | 1 |
| CF3Br (H1301) – Bromotrifluoromethan e | 0.5 | 1 | 0.5 | 0.5 | 0.5 | 0.5 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| CF2ClBr (H1211) – Bromochlorodifluorom ethane | 0.5 | 1 | 0.5 | 0.5 | 0.5 | 0.5 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| HNO3 - Nitric Acid | 1 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |

| Geophysical Variable | Images | Geographic Coverage | Horizontal Resolution | Temporal Refresh | Data Latency | Vertical Resolution | Precision: Clear/ Cloudy, Land/ Ocean | Accuracy | Validity Range | Long- term Stability | Robustness | Continuity |
|----------------------------------|--------|------------------------|--------------------------|---------------------|-----------------|------------------------|--|----------|----------------|-------------------------|------------|------------|
| N2O5 – Dinitrogen Pentoxide | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| H2O2 – Hydrogen Peroxide | 0.5 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| HCl – Hydrogen Chloride | 1 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| ClONO2 – Chlorine Nitrate | 1 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| ClO - Chlorine Monoxide | 0.5 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| OClO – Chlorine Dioxide | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| HF - Hydrogen Fluoride | 0.5 | 1 | 0.5 | 0.5 | 0.5 | 0.5 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| HNO4 – Peroxynitric Acid | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| HOCl – Hypochlorous Acid | 0.5 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| NO3 – Nitrate | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| NO2 – Nitrogen Dioxide | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| NO – Nitrogen Oxide | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| CH3OOH – Methyl Hydroperoxide | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| CO – Carbon | 0.5 | 1 | 0.5 | 0.5 | 0.5 | 0.5 | 0.8 | 1 | 1 | 1 | 1 | 1 |

| Geophysical Variable | Images | Geographic Coverage | Horizontal Resolution | Temporal Refresh | Data Latency | Vertical Resolution | Precision: Clear/ Cloudy, Land/ Ocean | Accuracy | Validity Range | Long- term Stability | Robustness | Continuity |
|-------------------------------------|--------|------------------------|--------------------------|---------------------|-----------------|------------------------|--|----------|----------------|-------------------------|------------|------------|
| Monoxide | | | | | | | | | | | | |
| HBr – Hydrogen Bromide | 1 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| BrO – Bromine | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| BrONO2 – Bromine Nitrate | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| HOBr – Hypobromous Acid | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| BrCl – Bromine Chloride | 0.5 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Cl2 – Chlorine | 0.5 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Aerosol Optical Depth | 1 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| Aerosol Layer Height | 1 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| Aerosol Single Scattering Albedo | 0.2 | 1 | 1 | 0.5 | 0.5 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| Aerosol Refractive Index | 0.2 | 1 | 1 | 0.5 | 0.5 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| Aerosol Particle Size | 0.2 | 1 | 1 | 0.7 | 0.7 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| Aerosol Particle Shape | 0.2 | 1 | 1 | 0.5 | 0.5 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| Speciated Aerosol Mass | 1 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |

| Geophysical Variable | Images | Geographic Coverage | Horizontal Resolution | Temporal Refresh | Data Latency | Vertical Resolution | Precision: Clear/ Cloudy, Land/ Ocean | Accuracy | Validity Range | Long- term Stability | Robustness | Continuity |
|-------------------------------|--------|------------------------|--------------------------|---------------------|-----------------|------------------------|--|----------|----------------|-------------------------|------------|------------|
| Volcanic Ash | 1 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| H2O - Water Vapor | 1 | 1 | 1 | 1 | 0.8 | | 0.8 | 1 | 1 | 1 | 1 | 1 |
| SO2 - Sulfur Dioxide | 1 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| SF6 - Sulphur Hexafluoride | 0.5 | 1 | 0.5 | 0.5 | 0.5 | 0.5 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| OH – Hydroxyl Radical | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |
| HO2 – Hydroperoxy Radical | 0.5 | 1 | 1 | 1 | 1 | 1 | 0.8 | 1 | 1 | 1 | 1 | 1 |

Sources of Stratospheric Composition Observational Needs:

The Core-SAT team, composed of federal employees from NOAA (including representatives from the NWS, NOAA OSAAP Analysis Team, and the NOAA LEO and GEO Programs), reviewed the air quality monitoring and forecasting observational needs by assessing the users' needs as developed by the SAT air quality subgroup, but also with the findings from other sources including:

- "A Value Assessment of an Atmospheric Composition Capability on the NOAA Next-Generation Geostationary and Extended Orbits (GEO-XO) Missions." DOI: <u>https://doi.org/10.25923/1s4s-t405</u>, https://repository.library.noaa.gov/view/noaa/27224
- "Chemical data assimilation estimates of continental U.S. ozone and nitrogen budgets during the Intercontinental Chemical Transport Experiment–North America." DOI: https://doi.org/10.1029/2006JD007722
- "A revised linear ozone photochemistry parameterization for use in transport and general circulation models: multi-annual simulations." DOI: <u>https://doi.org/10.5194/acp-7-2183-2007</u>
- "Tropospheric chemistry in the Integrated Forecasting System of ECMWF." <u>https://doi.org/10.5194/gmd-8-975-2015</u>
- Community of Practice, product baseline, and user value chain coordination through the User Engagement Council
- "Global Atmospheric Composition Needs from Future Ultraviolet–Visible–Near-Infrared (UV–Vis–NIR) NOAA Satellite Instruments" https://journals.ametsoc.org/view/journals/bams/104/3/BAMS-D-22-0266.1.xml

All these user needs were incorporated into this document, using a prioritized, vetted list of variables, with an agreed upon format (e.g., choice of units, etc.). This will allow for a better understanding of the overall needs for the air quality monitoring and forecasting application, a streamlining of the process to collect observational needs, and minimizing the outreach to users. The requirements' ranges, and their associated priorities, will also serve as an input to the ASPEN tool, which is used to assess potential future architecture solutions and their abilities to meet users' needs.

Important note: This memo was developed by the Subcommittee and approved after deliberations and discussions among the core-SAT, which consist of federal employees only. These recommendations were made following extensive scientific fact-finding, review of the scientific literature, and SAT discussions with scientific experts and others knowledgeable in the field.

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List of Acronyms

| Abbreviation | Definition | | | | | | | |
|--------------|---|--|--|--|--|--|--|--|
| | | | | | | | | |
| ARL | Air Resources Laboratory | | | | | | | |
| ASPEN | Advanced Systems Performance Evaluation tool for NOAA | | | | | | | |
| BAMS | Bulletin of the American Meteorological Society | | | | | | | |
| COURL | Consolidated Observational Users Requirements List | | | | | | | |
| СРО | Climate Program Office | | | | | | | |
| CSL | Chemical Sciences Laboratory | | | | | | | |
| DAAS | Deputy Assistant Administrator for Systems | | | | | | | |
| DoD | Department of Defense | | | | | | | |
| ECMWF | European Centre for Medium-Range Weather Forecasts | | | | | | | |
| EMC | Environmental Monitoring Center | | | | | | | |
| EPA | [U.S.] Environmental Protection Agency | | | | | | | |
| GEO | Geosynchronous Earth Orbit | | | | | | | |
| GeoXO | Geostationary Extended Observations (Previously GEO-XO) | | | | | | | |
| GML | Global Monitoring Laboratory | | | | | | | |
| IR | Infrared | | | | | | | |
| LEO | Low Earth Orbit | | | | | | | |
| NASA | National Aeronautics and Space Administration | | | | | | | |
| NESDIS | National Environmental Satellite, Data, and Information Service | | | | | | | |
| NOAA | National Oceanic and Atmospheric Administration | | | | | | | |
| NWS | National Weather Service | | | | | | | |
| OAR | Office of Oceanic and Atmospheric Research | | | | | | | |
| OBS | NWS Office of Observations | | | | | | | |
| OSAAP | Office of System Architecture and Advanced Planning (NOAA/NESDIS) | | | | | | | |
| OSCAR | Observing Systems Capability Analysis and Review tool | | | | | | | |
| RAQMS | Real-time Air Quality Modeling System | | | | | | | |
| SAT | System performance Assessment Team | | | | | | | |
| STAR | Center for Satellite Applications and Research | | | | | | | |
| SWO | Space Weather Office | | | | | | | |
| TPIO | Technology, Planning and Integration for Observation | | | | | | | |
| UV | Ultraviolet | | | | | | | |
| Vis | Visible | | | | | | | |
| WMO | World Meteorological Organization | | | | | | | |
| XORWG | GeoXO Requirements Working Group | | | | | | | |