

Exploring the Future of Infrared Sounding

Outcomes of a NOAA/NESDIS Virtual Workshop

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NOAA Infrared Sounder Workshop

What: The NOAA Infrared Sounder Workshop, held online in December 2021, brought together over 125 people from industry, academia, government, and research organizations from around the world to share information about the application of infrared (IR) sounders on polar-orbiting satellites in meteorology and atmospheric chemistry, and to provide recommendations on future generation sensor capabilities.

When: 6 December 2021

Where: Online (www.nesdis.noaa.gov/events/noaa-infrared-sounder-workshop)

KEYWORDS: Infrared radiation; Remote sensing; Satellite observations; Soundings

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Radiances from hyperspectral infrared (IR) sounders on board polar-orbiting satellites in low-Earth orbit (LEO) provide critical inputs to numerical weather prediction (NWP) to improve the initial conditions of atmospheric temperature and water profiles for forecasts. Additionally, hyperspectral IR soundings are used for retrieving atmospheric gases. The current operational hyperspectral IR sounders used in weather and atmosphere chemistry applications include the Atmospheric Infrared Sounder (AIRS) operated by the National Aeronautics and Space Administration (NASA), the Infrared Atmospheric Sounding Interferometers (IASIs) operated by the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT), and the Cross-track Infrared Sounder (CrIS) operated by the National Oceanic and Atmospheric Administration (NOAA). Geostationary satellites also carry hyperspectral IR sounders, like the Geosynchronous Interferometric Infrared Sounder (GIIRS) on the Chinese Meteorological Agency (CMA) *FY-4A* geostationary satellite. In addition, EUMETSAT will fly a hyperspectral IR sounder (IRS) on its Meteosat Third Generation (MTG) geostationary satellite launching in late 2023. NOAA is conducting formulation studies for a new IR sounder that could be hosted on its next generation geostationary satellite mission (GeoXO), a ground-breaking undertaking that will expand Earth observations from the GOES-R series. Menzel et al. (2018) provides an excellent history of IR sounders, including current capabilities and applications.

Hyperspectral IR sounders currently flown on polar-orbiting satellites make measurements in the 3–15.5 μm region of the electromagnetic spectrum, which cover the shortwave (SWIR; 3.6–4.64 μm ; 2,700–2,155 cm^{-1}), midwave (MWIR; 5.71–8.26 μm ; 1,750–1,219 cm^{-1}), and longwave (LWIR; 9.13–15.5 μm ; 1,095–640.2 cm^{-1}) regions of the IR spectrum. Figure 1 shows the spectral coverage of these sensors and absorption features of major atmospheric components of the IR spectra. The vibration and rotation of carbon dioxide (CO_2) molecules in the LWIR wavelengths region of 12.9–14.7 μm (770–680 cm^{-1}) and MWIR region of 4.16–4.54 μm (2,200–2,400 cm^{-1}) are primarily used for atmospheric temperature retrievals. Water (H_2O) molecule absorption in the MWIR region of 6.5–7.6 μm (1,500–1,300 cm^{-1}) is used for water vapor retrieval. Additionally, several molecules and physical parameters absorb in the thermal infrared enabling the inference of a rich suite of geophysical variables (e.g., Worden et al. 2006; Clerbaux et al. 2009; Kahn et al. 2014).

The NOAA Infrared Sounder Workshop

While the NOAA–NASA Joint Polar Satellite System (JPSS) and EUMETSAT’s MetOp satellites are expected to continue providing hyperspectral IR sounder measurements well into the next decade, NOAA is exploring mission concepts to complement and augment the current operational missions with new IR sounders, and is beginning preformulation studies for the next generation of IR sounders after CrIS. About two decades of hyperspectral IR sounder data are available starting with NASA AIRS, launched in 2002. The experience gained in exploiting this extensive data record provides a unique opportunity for NOAA and other weather satellite operators to assess the impact, utility, and quality of these data when planning and designing future IR sounders.

The NOAA LEO satellites program office hosted a virtual workshop on 6 December 2021 to seek inputs and recommendations in future mission planning. The workshop

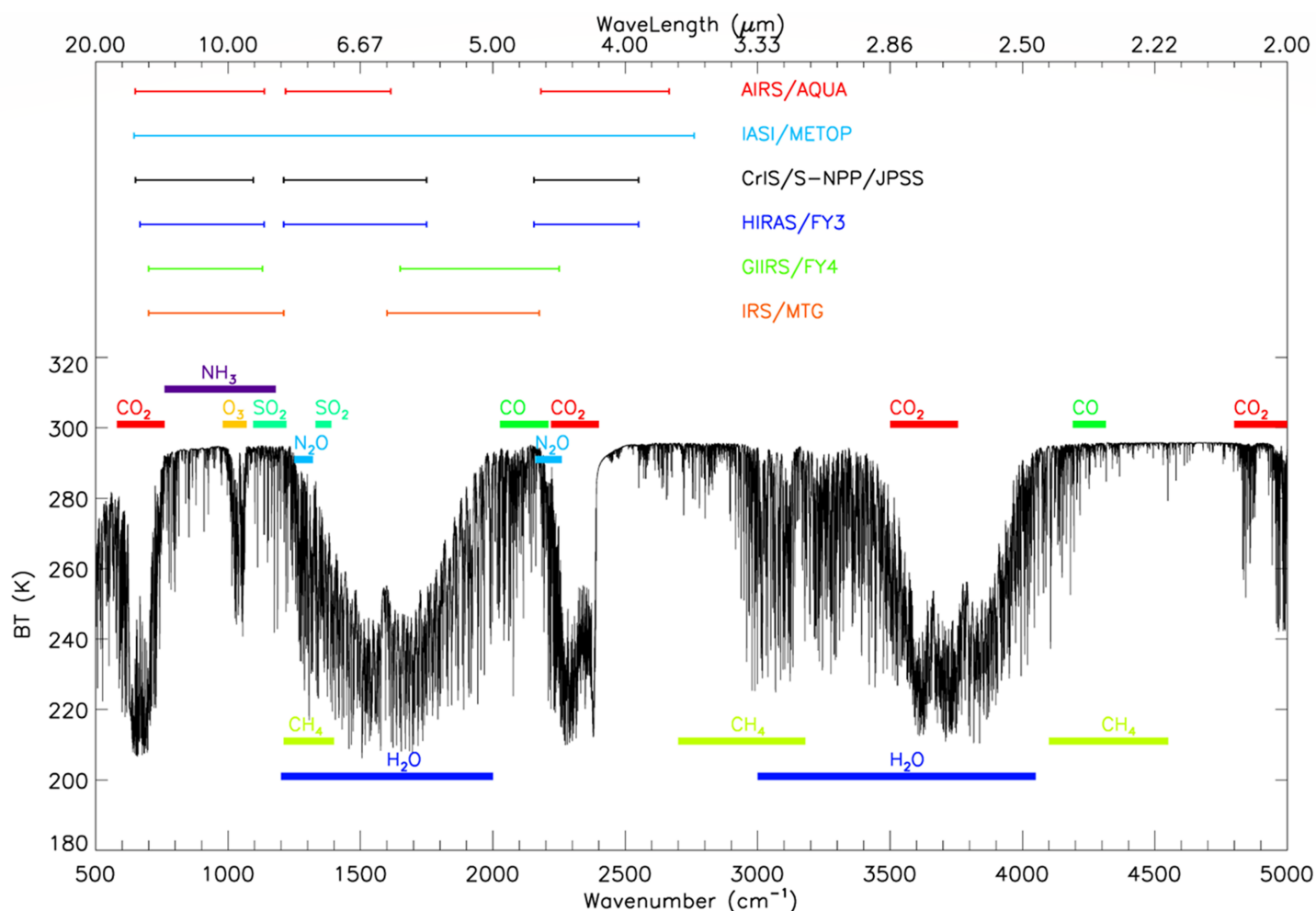


Fig. 1. Atmospheric absorption features in the infrared region of the electromagnetic spectrum. (Courtesy: Yong Chen, STAR, NOAA/NESDIS.)

was attended by over 125 people from industry, academia, government, and research organizations. Global experts in meteorology and atmospheric chemistry presented their perspectives on the applications and needs of IR sounders, and participants discussed measurement use and importance, required capabilities, and desired improvements. Presenters included Kevin Bowman (Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California), Cathy Clerbaux (LATMOS/Institut Pierre-Simon Laplace, CNRS, France), Andrew Collard (National Centers for Environmental Prediction, National Weather Service, NOAA), John Eyre (Met Office, United Kingdom), Greg Frost (Oceanic and Atmospheric Research, NOAA), Norio Kamekawa (Japan Meteorological Agency), Gregory Mandt (JPSS/NOAA), Tony McNally (European Centre for Medium-Range Weather Forecasts), William McCarty (Global Modeling and Assimilation Office, NASA), Kazuyuki Miyazaki (Jet Propulsion Laboratory, California Institute of Technology, Pasadena), Bradley Pierce (SSEC, University of Wisconsin–Madison), Kaitlin Rutt (National Weather Service, NOAA), Fiona Smith (Bureau of Meteorology, Australia), and William Smith Sr. (SSEC, University of Wisconsin–Madison). Presentations can be found on the NOAA/NESDIS website (www.nesdis.noaa.gov/events/noaa-infrared-sounder-workshop). A high-level overview of workshop findings is provided here.

Current uses and applications of IR soundings of Earth's atmosphere

Bringing together the atmospheric science community provided the opportunity to learn about end user applications and the importance of IR sounding measurements to meet user

objectives. Feedback from participants about the utility, advantages, and limitations of IR sounders is summarized below.

IR soundings in data assimilation for numerical weather prediction. Data denial experiments have shown that microwave (MW) sounders and imagers have the largest impact in reducing forecast errors, as these observations can be used in the presence of clouds through all-sky schemes, and also partly because more MW sensors are operating compared to IR sounders (Saunders 2021). However, hyperspectral IR satellite data are the largest percentage of observations assimilated into NWP models (e.g., Bormann et al. 2019). Hyperspectral IR data have the potential to deliver much higher-vertical-resolution information than a microwave instrument. In recent years, Forecast Sensitivity-based Observational Impact (FSOI) assessments have shown that MW and IR soundings have similar impacts per observation (Fig. 2). Either directly measured radiances or radiances that are reconstructed from principal component analysis (PCA) from IR sounders are directly assimilated into NWP models.

Successfully controlling cloud contamination is critical for exploiting IR soundings. Because the radiative transfer physics of the atmosphere are different between IR and MW measurements, the techniques for screening and resolving cloud-affected observations are also different. There are large uncertainties in forward modeling of cloudy IR radiances, and techniques have progressed from assimilating cloud-free radiances (fully clear scenes) and radiances over completely overcast regions (McNally 2009), to more aggressive approaches that use channels with most sensitivity above the cloud top (Pavelin et al. 2008). Nonetheless, several NWP centers routinely assimilate clear and completely cloudy scenes only.

While there are over 2,000 spectral bands in modern IR sounders, typically a few hundred channels are selected with a subset assimilated into NWP (“thinning”). Using fewer channels

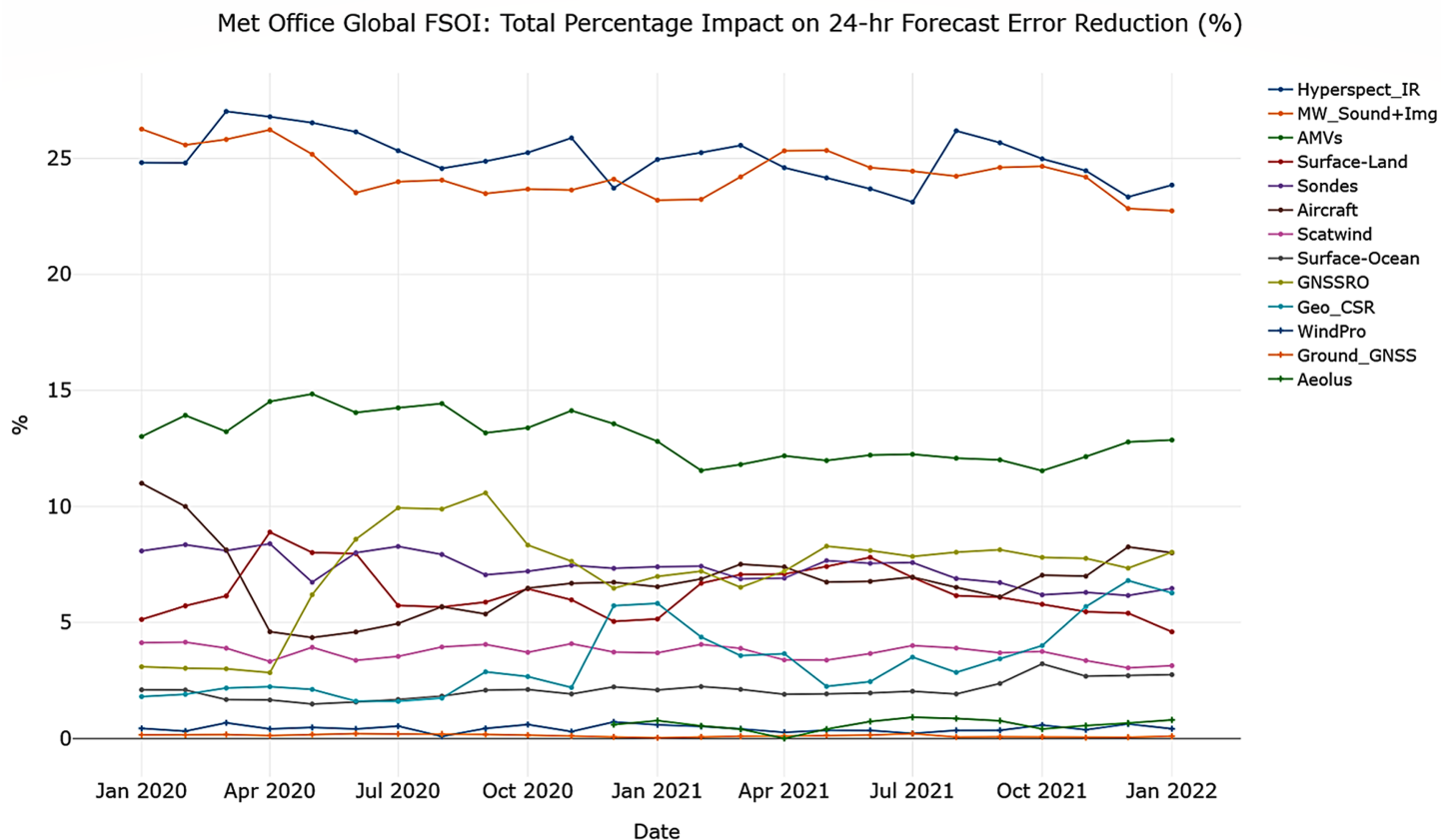


Fig. 2. Forecast Sensitivity-based Observational Impact (FSOI) assessments of various observations on 24 h forecast error reduction at the Met Office, over a 2-yr period (2020–22). (Courtesy: John Eyre, Met Office.)

Table 1. CrIS instrument information content (IC)/degrees of freedom (DOF) for temperature and humidity for various assumed spectral channel combinations and noise levels associated with optimal estimation profile retrieval or NWP model radiance assimilation. Boldface text indicates that the spectral band combinations and noise levels provide a large amount of the CrIS radiance IC. Italicized text indicates that they provide a moderate amount of CrIS IC. Plain text (not boldface or italicized) denotes a small amount of the CrIS IC provided for NWP data assimilation purposes. (Courtesy: Bill Smith Sr., UW SSEC.)

CrIS bands	All	LW + MW	MW + SW	LW	MW	SW
Temperature: Shannon IC	34.4	33.6	19.7	32.4	14.7	13.9
Humidity: Shannon IC	32.0	32.0	29.6	14.5	<i>29.1</i>	4.2
Temperature: DOF	10.1	9.8	<i>6.3</i>	9.6	4.1	<i>5.5</i>
Humidity: DOF	6.5	6.4	5.5	2.8	5.2	1.3

minimizes data volume and the impacts of other chemical species that affect temperature and water vapor measurements. For example, ECMWF assimilates about 220 IASI channels in their NWP systems. Two methods are used together for cloud detection within IASI scenes at ECMWF: the first is an algorithm that identifies the characteristic signal for cloud presence in IASI observed backgrounds (O-Bs), and channels not affected by clouds are assimilated; the second method relies on a cloud mask produced by the Advanced Very High Resolution Radiometer (AVHRR). To eliminate cloud cover and observational biases from horizontal observational errors at different scan positions, the number of fields of view (FOV) in a field of regard (FOR) are further limited in global NWP data assimilation (DA). For example, out of the 3×3 FOVs in a CrIS FOR, only one FOV is currently selected for assimilation in global NWP models. At the NWS National Centers for Environmental Prediction (NCEP), 431 CrIS channels are selected out of the available 2,211 CrIS channels (Noh et al. 2021). Within this subset, about 100 are routinely assimilated, which are spread around the $650\text{--}780\text{ cm}^{-1}$ ($15.34\text{--}12.82\text{ }\mu\text{m}$) LWIR region for temperature sounding, $1,300\text{--}1,600\text{ cm}^{-1}$ ($7.6\text{--}6.2\text{ }\mu\text{m}$) MWIR for water vapor sounding, and $650\text{--}780\text{ cm}^{-1}$ ($15.3\text{--}12.822\text{ }\mu\text{m}$) LWIR window channels for surface sensing. Although using fewer channels reduces the data volume and the number of time-consuming forward radiative transfer model radiance calculations, it significantly reduces the information content of these data (Smith et al. 2021). Spatial data sampling thinning also reduces the data volume, but this can act to degrade the forecast impact of the data since convective initiation and precipitation processes are related to small-spatial-scale variations in atmospheric humidity. The negative impacts of using channel selection and spatial sampling data thinning can be alleviated by using PCA for data compression as currently employed by IASI, and a spectrum-based, rather than a channel-based, radiative transfer model for the radiance data assimilation.

Longwave + midwave (LW + MW) IR sounding channels have the highest information content and are the only channels currently used in NWP DA. Table 1 shows the CrIS instrument information content (IC) and degrees of freedom (DOF) for temperature and humidity based on the Nyquist–Shannon sampling theorem: the resolution of features within a continuous time/frequency signal of finite bandwidth increases with the number of discrete measurements (e.g., a vertical profile feature sensed by a spectrum of radiances) (Smith et al. 2021).

While these results are for an ideal case where the Jacobians of temperature and water vapor are precisely known, and where observational errors are well characterized, this analysis of relative IC and DOFs among the three IR wavelength regions is still relevant. SW IR sounding channels are not currently assimilated in NWP models partly because of the nonlocal thermodynamic equilibrium of the atmosphere where the exchange of energy between CO_2 molecules from vibration and collision is not well defined. Also, daytime solar reflection, interfering atmospheric species, and higher noise impedes SW data assimilation compared to other wavelengths. While basic research to assimilate SW radiances in NWP is ongoing, early results show mixed

results. Much of the DA is adaptive and autonomous (i.e., adjustments to model state at various times and locations, bias corrections of observations, models, and background random errors are done without human intervention), but new sensors require significant human resources. Due to resource limitations, problematic sensors are sometimes ignored; users rely on stable and well understood sensors and calibration stability is very important.

Studies show that observations located near the end of the assimilation time window are significantly more influential than observations at the start of the window (McNally 2019). High timeliness [e.g., via direct broadcast network (DBNet)] is therefore valuable since it allows the most recent observations to be used in NWP models within the assimilation cutoff window.

Frequent IR measurements of water vapor enable tracking of atmospheric motion vectors (AMV). The utility of using atmospheric sounders to perform feature tracking for retrieval of AMVs has been investigated using the AIRS instrument over the poles where orbital coverage occurs every 55 min. These AMVs fill a midtropospheric data gap from the Moderate Resolution Imaging Spectroradiometer (MODIS) and AVHRR-derived AMVs. AMVs derived from IR sounders in polar regions are not yet operationally assimilated at NWP centers.

The concept of assessing the impact of individual satellite observations on severe weather prediction, like tropical cyclones, is a widely understood approach to inform agencies on mission impacts and future formulation. However, impact assessments are expensive and time consuming and very few cyclones exist in any given test period, making it challenging to complete a robust quantitative assessment.

IR soundings in retrievals of atmospheric profiles. In addition to assimilating IR sounding data into NWP models, the data are also used with MW soundings for retrievals of vertical profiles of temperature, water vapor ozone (O_3), and trace gases [carbon monoxide (CO), methane (CH_4), CO_2 , volcanic sulfur dioxide (SO_2), nitric acid (HNO_3), and nitrous oxide (N_2O)] using systems like the NOAA Unique Combined Atmospheric Processing System (NUCAPS) (Kalluri et al. 2022). The NUCAPS temperature and water vapor profiles are used by NWS forecasters in the Advanced Weather Interactive Processing System (AWIPS) for environmental analysis to supplement model outputs and conventional radiosonde observations, and for visual analysis of spatially gridded profiles to determine atmospheric instability for now-casting applications.

Atmospheric chemistry. The four most important greenhouse gases resulting from anthropogenic activities are CO_2 , CH_4 , N_2O , and O_3 . Changes in thermal absorption of these radiatively active gases are the fundamental drivers of climate change. Hyperspectral IR sounders provide valuable supplemental measurements for atmospheric chemistry applications in the following wavelengths: SWIR (CO , CO_2), MWIR (N_2O , CH_4), and LWIR (CO_2 , O_3). The IR wavelengths of most interest for atmospheric chemistry where the vibration and rotation of molecules lead to absorption include the following:

- 2.2, 3.3, and 7.6 μm for CH_4
- 2.3 and 4.6 μm for CO
- 4.5 and 7.9 μm for N_2O
- 7.34 μm for SO_2
- 9.6 μm for O_3
- 4.3 and 15 μm for CO_2

IR sounders such as AIRS, CrIS, Tropospheric Emission Spectrometer (TES), and IASI have played a fundamental role in understanding chemistry–climate interactions. They provide good augmentation to other sensors since they sample most of the troposphere, which is

relatively under-sampled. The IR sounders complement other missions dedicated to atmospheric chemistry, including the Tropospheric Monitoring Instrument (TROPOMI), Ozone Monitoring Instrument (OMI), the *Orbiting Carbon Observatory-2* (OCO-2), Ozone Mapping and Profiler Suite (OMPS), the Global Ozone Monitoring Experiment-2 (GOME-2), and the *Greenhouse Gas Observing Satellite* (GOSAT), which make measurements in ultraviolet–visible (UV–vis) and near-IR (NIR) regions. Panspectral techniques provide better vertical sensitivities than individual bands because they sample at different levels in the atmosphere, which is critical for relating concentrations to emissions (Worden et al. 2007; Landgraf and Hasekamp 2007; Cuesta et al. 2013; Fu et al. 2018). For example, ozone as seen by CrIS (or IASI and GOME-2) is a mixture of both tropospheric and stratospheric processes; however, CrIS and TROPOMI together provide better vertical distribution of ozone (Mettig et al. 2022). Thermal IR observations are sensitive to the free-tropospheric trace gases, whereas UV–vis–NIR observations are sensitive to the column abundances of trace gases. However, the ability of IR sounders to probe the planetary boundary layer, where local pollution occurs, strongly depends on location, temperature, type of surface, and time of the day (Clerbaux et al. 2009).

Unlike NWP models that directly assimilate radiances, applications in atmospheric chemistry DA rely mainly on retrievals based on techniques, such as optimal estimation, machine learning, and neural networks (Rodgers 2000), and need additional parameters, like quality control flags, a priori, and averaging kernels, to effectively assimilate the retrievals into atmospheric models while reducing DA computational costs (Jones et al. 2003; Pierce et al. 2007; Migliorini et al. 2008). The science community expects these tools for rigorous science and assimilation of remote sensing data. The NASA Global Modeling and Assimilation Office (GMAO) conducted experiments to assimilate IR radiances in the 9.6 μm ozone band from CrIS, AIRS, and IASI in the Goddard Earth Observing System (GEOS) model. The results show improved resolution of tropical wave one ozone maximum (WOOM) signal at 300 hPa (Solomon et al. 2005; Jenkins et al. 2021). These changes reduced systematic errors against ozonesondes. Many NWP centers assimilate ozone channels operationally.

Finally, there are numerous successful applications of atmospheric chemistry measurements from IR sounders, including measuring volcanic hydrogen sulfide (H_2S) and SO_2 , wildfire emissions of CO, O_3 , ammonia (NH_3), volatile organic compounds (methanol, formic acid, etc.) and peroxyacyl nitrates (PANs), monitoring changes in the ozone hole (O_3 and HNO_3) over Antarctica, monitoring agricultural practices using NH_3 observations (Van Damme et al. 2018), and detecting concentration changes during COVID-19 lockdowns (Miyazaki et al. 2021). Figure 3 provides an example of fire emissions retrieved by CrIS during the historic 2020 California wildfires. Atmospheric chemistry measurements from IR sounders are routinely used in several operational monitoring systems, including the Copernicus Atmospheric Monitoring Service (CAMS), Copernicus Climate Change Service (C3S), the JPL Multi-model Multi-constituent Chemical data assimilation (MOMO-Chem), Total Ozone from Analysis of Stratospheric and Tropospheric components (TOAST), and the Real-time Air Quality Modeling System (RAQMS).

Recommendations for future NOAA IR sounders

The NOAA workshop provided excellent discussion about how the atmospheric science community uses IR sounding measurements. The community provided a broad array of suggestions to address needs and desired improvements. Discussions touched on ideal configurations, additions to existing capabilities, and other factors related to the impact of IR soundings. Key takeaways and recommendations are presented below.

Maintain the backbone of LEO observations. Maintaining the backbone of LEO observations with highly capable sensors like CrIS and IASI is critical. MW and LW bands are the foundation for NWP models and SWIR/NIR is the foundation for carbon species (CO_2 , CO, CH_4) observation.

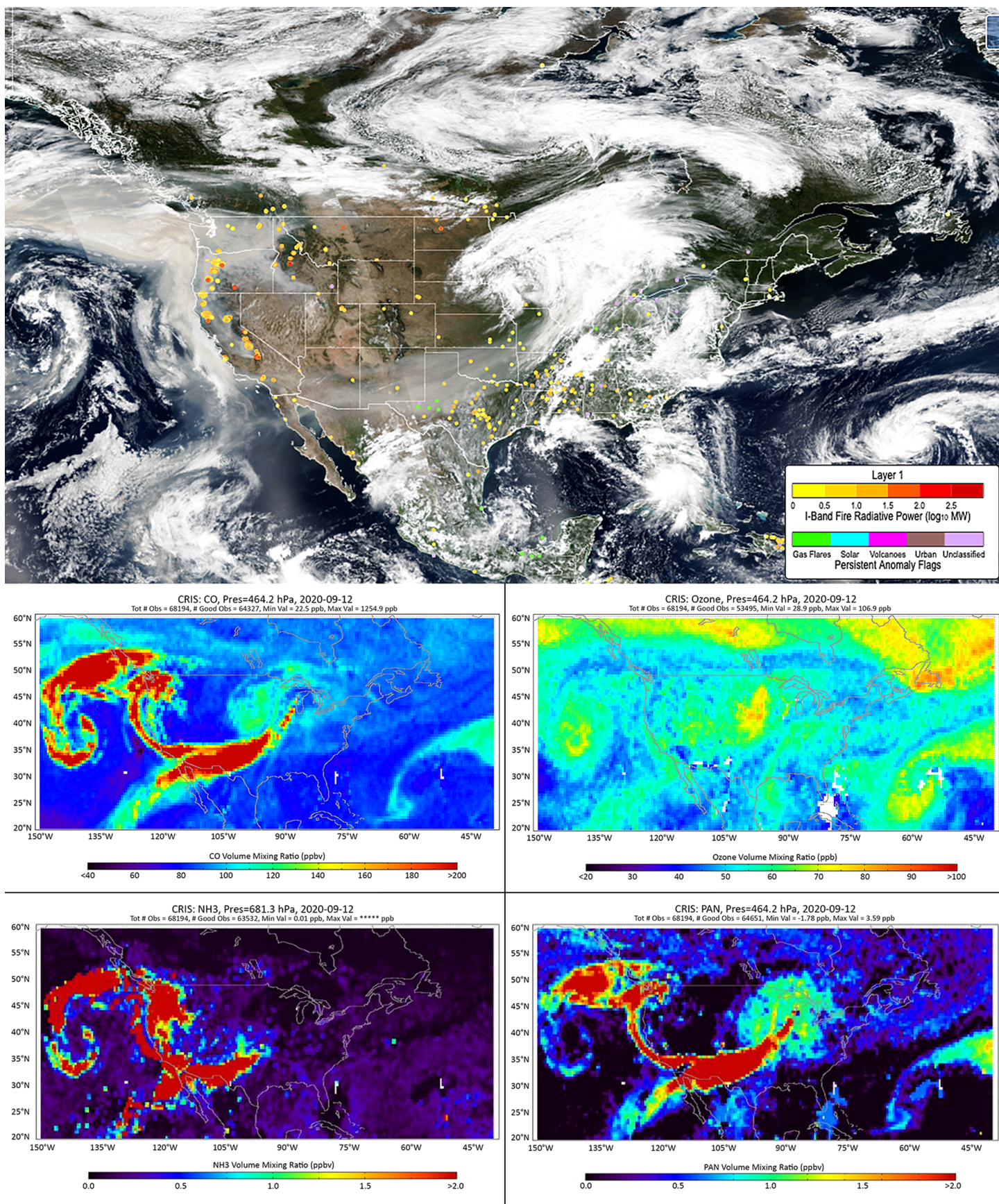


Fig. 3. (top) True color image from the Visible Infrared Imaging Radiometer Suite (VIIRS) showing fires over California on 12 Sep 2021 and (middle) CO and O₃ and (bottom) NH₃ and PAN retrieved by CrIS. (Courtesy: Kevin Bowman, NASA JPL.)

Maintaining a suite of sensors in the 1330 local time of the ascending node (LTAN) orbit with calibration accuracy, stability, traceability, swath width, and data quality comparable with current CrIS is important. Ideally, all supplemental orbit sensors should have these characteristics. However, additional measurements to augment the backbone could be operative at a higher noise level of measurement assuming that fixed instrument performance parameters (i.e., FOV size, spectral coverage, and spectral resolution that cannot be enhanced during ground data processing) meet the backbone requirements.

Consider noise characteristics. For the thermal IR observations, spectral resolution and noise provide bounds for both *what* and *where* vertical resolution is obtainable. While low noise is necessary, it should not come at the cost of other factors, such as spectral and spatial resolution. Noise equivalent delta temperature (NEDT) and spectral resolution should be considered together. Measurement noise should be as small as practically possible but should not be achieved at the expense of an instrument's unacceptably low spatial resolution. The impacts of single sample noise can be minimized by intelligent spatial averaging and optimal spectral convolution using techniques like PCA. Current standard deviation statistics of O-B monitoring demonstrated for key tropospheric temperature sounding channels is 0.1–0.2 K and for key tropospheric humidity sounding channels is ~1.0 K. The noise characteristics of future sounders should be equal to or better than these values. The combination of stable calibration over time and low noise are important for NWP applications and climate reanalysis studies. Future IR sounders should have onboard calibration with International System of Units (SI) traceability, like that of CrIS.

Improve the spatial resolution. Improved spatial resolution increases tropospheric sounding yield by 15%–60% (Smith et al. 2017). Sounding accuracy improves at the FOR level with higher-spatial-resolution FOVs due to decreased cloud contamination. Sounding accuracy is significantly more dependent on cloud contamination than it is on detector noise. Smaller FOV/ground space distance greatly increases FOR yield. Important spatial water vapor features are resolved with high-horizontal-resolution (2 km) radiance data. Higher-horizontal-resolution satellite data and forecast models provide more accurate convective weather precipitation forecasts.

Apodization. Data from Fourier transform spectrometers (FTS), like CrIS and IASI, are apodized to eliminate ringing artifacts in the FTS-derived radiance spectrum that arise from a finite path difference. The apodization, however, comes at the cost of reduced spectral resolution and introduces spectral correlation among adjacent channels. IASI L1C Gaussian apodization retains 70% of the first resonance and 20% of the second resonance, but CrIS Hamming apodization retains only 10% of the first resonance. Therefore, it is important to effectively remove the apodization, especially for CrIS, without sacrificing the information content.

Extend the shortwave range. Historically, polar-orbiting environmental satellites hosted multiple sensors, including a multipurpose visible–infrared imager (vis–IR), IR and MW sounders, and an ozone sensor, on the same spacecraft to allow simultaneous measurements in various regions of the electromagnetic spectrum. Colocation of IR sounders with MW sounders and vis–IR imagers is desirable but not essential for NWP applications. However, panspectral approaches, like collocation with SWIR/NIR (O_3 , CO_2 , CO , CH_4), are *essential* for near-surface resolution for atmospheric chemistry. The complementarity of thermal IR (TIR) and SWIR will allow more information on the vertical distribution of trace gases such as CO_2 , CH_4 , and CO . TIR instruments lack sensitivity to the surface when thermal contrast (temperature difference between the ground and the air just above) is low, and SWIR

instruments only provide total columns. In the future, the SW range of IR sounders should be extended to 1.5–2.5 μm since this range is required to retrieve the entire total tropospheric column of CO , CO_2 , and CH_4 . Spectral range and resolution matter—the higher the resolution, the better the measurement.

Continue twice-daily measurements in sun-synchronous orbits. The combination of morning and afternoon orbits capture the evolution of the photochemical processes. Afternoon orbits provide measurements during peak solar illumination and human activity for air quality forecasts, especially for short-lived species in the troposphere. Therefore, twice-daily atmospheric chemistry measurements in sun-synchronous orbits should continue.

Improve the spectral resolution to meet next generation requirements. Next generation IR sounders, such as IASI-NG (Crevoisier et al. 2014), will have improved spectral resolution of 0.25 cm^{-1} compared to IASI at 0.5 cm^{-1} and CrIS at 0.625 cm^{-1} . At a minimum, future IR sounders should have spectral resolution that is equal to or better than 0.625 cm^{-1} without gaps in the spectra. Increasing the spectral and spatial resolution will lead to higher data volumes. To reduce the data volume, increasing onboard data processing like the approach for IASI could be considered, as well as transmitting the principal components of the spectra for assimilation.

In summary, the NOAA workshop demonstrated that users from industry, academia, government, and research organizations have a broad range of needs and interest in the next generation of IR sounders. The workshop was successful in providing ample user feedback that can be applied to future development. Considering its success, NOAA intends to organize similar workshops for other Earth observation instruments.

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