SOFIE Version 1.3 (V1.3) Data Description.

V1.3 changes that affected all observations are described below.

Level 0 Changes:

- None.

Level 1 Changes:

- A non-linear least squares fit was used to capture using high order components in SOFIE signal drift, to provide more robust signal drift corrections. The high order correction (HOC) contains up to third order terms and a sinusoidal component (amplitude, phase, frequency). The HOC functions were derived for each of the 16 bands, by characterizing the exo-atmospheric portion of many SOFIE events (spanning the entire mission to date). Sunrise and sunset events are handled independently in the HOC approach. The individual HOC terms can employ weighted taper functions in altitude, depending on the specific band characteristics. See Table 2 for specific information on the signal corrections.
- Changes in the AIM orbit caused the SOFIE attenuator balance to occur at increasingly low altitudes from early April 2015 on. This change caused difficulties in L1 processing that were rectified by adjusting signal levels for the balance portion of each event. This special processing will occur for events from April 2015 until SOFIE operations corrects this issue (estimated by September 2015).
- Created a new approach for Level 1 signal averaging, which is used to reduce the noise level prior to retrieval. This tactic is designed primarily for retrievals of meteoric smoke extinction, and to allow CO_2 retrievals to extend to higher altitude. Use of this method will eventually lead to public release of the SOFIE smoke and CO_2 data products.
- The interface to the NRL2000 MSIS model was updated. A sporadic bug in the reporting of event longitudes was fixed.

Level 2 Changes:

- CO_2 used in temperature / pressure (T/P) retrievals is now from a climatology based on a new version of WACCM (ref 2c). Atomic O is from a climatology based on SABER measurements, this impacts the quenching of excited states of CO_2 and is important in the band 13 radiance model. Primary impact is on T/P but through density this can impact retrieved gas VMR.
- V1.3 includes modifications to allow use of averaged Level1 signals. Increased the altitude range of Level 2 processing to take advantage of higher Signal/Noise ratios of averaged Level 1 Data.
- V1.3 retrieval precision values are reported as variances, where V1.2 reported standard deviations. Taking the square root of the V1.3 variances will yield values equivalent to the standard deviations in V1.2. SOFIE precision values are the sensitivity determined in the retrieval iteration process. These values are overly optimistic and should not be used. Rather, the data user should refer to the relevant SOFIE validation papers.

V1.3 changes and status specific to individual data products are described in Table 1, including summaries of the product altitudes (reported and endorsed for scientific use), and current validation status. Note that SOFIE reports missing data as -1e30 (or -1e24). In some cases values of 1e-14 will appear (mostly in aerosols or NO). These are when there was a good signal but no retrieval was possible (e.g., because the interference was larger than the measured signal).

Table 1. SOFIE Version 1.3 Data Description			
Product Measurement (Wavelength)	**Altitudes**[1]	**Validation**[2]	**Status**[3]
Temperature band 13 (4.324 μm) refraction (0.701 μm)	Endorsed: 15 - 88 km Reported: 10 - 102 km	*Stevens et al.* [2012], compared SOFIE V1.2 to SABER and ACE. For polar summer in the SH, SOFIE V1.3 is within 2 K of SABER for altitudes below the mesopause. For polar summer in the NH, SOFIE V1.3 is within 2 K of SABER for altitudes below ~80 km, with SOFIE up to 4 K warmer than SABER for ~80 to 90 km.	The SOFIE temperature (T) product is based on T retrieved from refraction angle measurements at altitudes from the tropopause to ~50 km, and T retrieved from the 4.324 μm CO_2 band at altitudes from ~50 km to ~100 km. V1.3 Level2 uses CO_2 from a recent version of WACCM, ref 2c, and atomic O from SABER climatology. These changes can impact retrieved T(P) significantly above 70km. Atomic O is important in the CO_2 NLTE model as it is one of the primary gases that quench excited states of CO_2. Compared to V1.2, V1.3 is similar below 70 km. At PMC heights V1.3 is ~0 to 4 K colder in the NH and 1 - 8 K colder in the SH. V1.3 also reports the T & P profiles extending to 150 km. Above the SOFIE T/P top altitude, these extended profiles are from WACCM model results merged to the SOFIE profile.
H_2O band 6 (2.618 μm)	Endorsed: 20 - 95 km Reported: 17 - 95 km	*Rong et al.* [2010], compared SOFIE V1.022 to MLS and ACE: within ~10% in the NH, SOFIE low by ~20% in the SH. SOFIE V1.3 is similar.	Compared to V1.2, V1.3 is similar in the SH and ~5% lower in the NH. As of V1.2, bands 5 and 6 have improved drift corrections, and an adjusted altitude window for the correction, which slightly reduced the systematic error at high altitudes. N_2O is now included in the forward model and this has removed a positive bias in the mid-to-lower stratosphere. Note that the SOFIE H_2O measurements are unaffected by PMC contamination.
O_3 band 1 (0.291 μm)	Endorsed: 55 - 95 km Reported: ~52 - 105 km	*Smith et al.* [2013], compared to SABER: within ~0.2 ppmv at 60 - 10 km. *Rong et al.* [in prep], compared to ACE: within ~1% for 55 - 93 km.	V1.3 is similar to V1.2, except above ~90 km where v1.3 is ~20% lower. As of V1.2, O_3 retrievals include a correction for PMC contamination as of V1.2, based on an extrapolation of the 0.330 μm wavelength extinctions to 0.291 μm. These corrections only occur from November 2009 to present, when the 0.330 μm band came out of saturation. The bottom altitude of the O_3 profiles is determined from the signal level, and can vary with season (~55 km on average). Note that the 0.291 μm O_3 band is completely opaque at lower altitudes.

CH_4 band 11 (3.384 µm)	Endorsed: 30 - 78 km Reported: 21 - 80 km	*Laeng et al.* [2015], compared to MIPAS: within 0.02 ppmv for 45-70 km. Occasional high bias in SOFIE below ~30 km.	V1.3 is similar to V1.2. The CH_4 retrievals are currently useful below ~78 km. At higher altitudes, the signal-to-noise is low, and the retrievals are contaminated when PMCs are present.
NO band 16 (5.316 µm)	Endorsed: 40 - 140 km Reported: 35 - 149 km	*Gomez-Ramirez et al.* [2013], compared to ACE at 97-106 km: within ~15% in the NH, SOFIE low by 5-35% in the SH. SOFIE is within 50% of HALOE for ~80 to 130 km (HALOE data several years prior to SOFIE).	V1.3 is similar to V1.2 in the SH, and ~20% higher in the NH. As of V1.2, Signal corrections are applied to remove a damped oscillation that is traced to varying detector temperatures. New in V1.3 SOFIE NO is also reported as number density profiles (molecules cm^{-3}). Both NH and SH data are available in daily L2 files and in mission files (see "data services on the SOFIE website). For scientific studies using SOFIE NO see *Baily et al.* [2014] and *Hendrickx et al.* [2015]. Note that due to the changing AIM orbit, NO retrievals were not accomplished from April 15 thru August 31 2015. The problem is solvable and NO for this period will be available in the future.
CO_2 band 7 (2.785 µm) band 13 (4.324 µm)	Endorsed: TBD Reported: TBD	Compared to WACCM: SOFIE low by ~5 ppmv in the NH, within ~1 ppmv in the SH	CO_2 retrievals were implemented in V1.2, independently using bands 7 and 13. The results are valid at altitudes where temperature is retrieved from refraction angle measurements (Z < ~55 km). CO_2 is not yet released to the public, because of occasional oscillations and anomalously high values (> 400 ppmv). Contact Mark Hervig (m.e.hervig@gats-inc.com) if you would like to receive the data for internal use.
UV Aerosol Extinction band 2 (0.330 µm)	Endorsed: PMC altitudes Reported: 17 - 95 km	Use of these measurements for PMCs is discussed in *Hervig et al.* [2012]. V1.3 PMC extinctions and resulting PMC properties are similar to V1.2.	The primary goal of this measurement is PMCs. Band 2 was saturated from launch until November 2009. By this point darkening of the optics had reduced the incoming UV light enough to bring the detector out of saturation. PMC extinction in band 2 is strong, and only slightly lower than the strongest IR bands (8 - 10).

NIR Aerosol Extinction bands 3 & 4 (0.867 & 1.037 µm)	Endorsed: PMC altitudes Reported: 17 - 95 km	V1.3 is ~10 to 40% greater than V1.2 at PMC altitudes in the NH.	The primary goal of these measurements is PMCs. The NIR extinctions, β(λ), can be very low, such that these measurements often do not respond to PMCs that are detected by the IR bands. While the NIR PMC extinction is best characterized using the high gain difference of bands 3 and 4 (channel 2), bright PMCs are well represented by bands 3 and 4. These measurements were used to characterize meteoric smoke in the upper stratosphere and mesosphere [*Hervig et al.*, 2009]. Note that this was accomplished by averaging the signals *before* retrieving extinction, in order to reduce the noise, and thus prevent a high bias in extinction when the transmissions are near unity. This step is required to use the extinctions for smoke studies.
NIR Aerosol Extinction channel 2 difference signal (extinction at 0.867 µm minus that at 1.037 µm wavelength)	Endorsed: PMC altitudes Reported: 41 - 110 km	Use of these measurements for PMCs is discussed in *Hervig et al.* [2009; 2012]. V1.3 PMC extinctions and resulting PMC properties are similar to V1.2.	The primary goal of this measurement is PMCs. This measurement is the difference of aerosol extinction at 0.867 µm minus that at 1.037 µm wavelength (band 3 - band 4). The difference signal experiences an electronic gain of 300, and thus is not digitization-limited like the component bands 3 and 4 measurements. Thus this is the recommended measurement for characterizing PMCs in the NIR. As of V1.2 the channel 2 dV extinction retrieval was reformulated to yield the exact 0.867 - 1.037 µm extinction difference. Previous versions used the theoretical ratio of 0.867/1.037 µm PMC extinction (2.0).
IR Aerosol Extinction band 5 (2.462 µm)	Endorsed: TBD Reported: 17 - 110 km	-	*This measurement is not recommended for scientific use.* The band 5 extinctions are typically biased high relative to expectations based on the other PMC measurements. This problem is thought to be due to gaseous interference that is not being removed correctly, and/or signal drifts that are not properly removed.
IR Aerosol Extinction band 8 (2.939 µm)	Endorsed: PMC altitudes Reported: 17 - 110 km	Use of these measurements for PMCs is discussed in *Hervig et al.* [2009] and *Hervig and Gordley* [2010]. V1.3 PMC extinctions and resulting PMC properties are similar to V1.2.	The primary goal of this measurement is PMCs. This wavelength has one of the highest PMC signals, as it is located near the peak of the OH-stretch region of the ice spectrum. This is an excellent measurement for characterizing PMCs.

IR Aerosol Extinction bands 9 & 10 (3.064 & 3.186 µm)	Endorsed: PMC altitudes Reported: 17 - 95 km	Use of these measurements for PMCs is discussed in *Hervig et al.* [2009; 2012] and *Hervig and Gordley* [2010]. V1.3 PMC extinctions and resulting PMC properties are similar to V1.2.	The primary goal of this measurement is PMCs. These wavelengths have the highest PMC signals of all of the SOFIE measurements. They were located near the peak of the OH-stretch region of the ice spectrum. These bands are used to identify PMCs in SOFIE profiles, and band 9 is the basis for determining ice mass density (and IWC). These are excellent measurements for characterizing PMCs.
IR Aerosol Extinction band 12 (3.479 µm)	Endorsed: PMC altitudes Reported: 17 - 110 km	V1.3 PMC extinctions are similar to V1.2.	The primary goal of this measurement is PMCs. Band 12 extinctions are consistent with the other observations, considering the wavelength dependence expected for PMCs.
IR Aerosol Extinction band 14 (4.646 µm)	Endorsed: TBD Reported: 17 - 110 km	-	*This measurement is not recommended for scientific use.* The band 14 extinctions are typically biased high relative to expectations based on the other IR measurements. This problem is thought to be due to gaseous interference that is not being removed correctly, or signal drifts that are not properly removed.
IR Aerosol Extinction band 15 (5.006 µm)	Endorsed: PMC altitudes Reported: 17 - 110 km	V1.3 PMC extinctions are similar to V1.2.	The primary goal of this measurement is PMCs. Band 15 extinctions are consistent with the other observations, considering the wavelength dependence expected for PMCs.
Aerosol Extinction in the stratosphere General statements for all bands.	Reported: > ~17 km	-	SOFIE reports aerosol extinctions for various wavelengths at altitudes from roughly 17 - 95 km. These results are currently not suitable for studies of the stratospheric aerosol layer. This limitation is due primarily to incomplete removal of gaseous interference, deficits in the signal drift corrections, and treatment of the FOV and solar refraction at low altitudes. While the deficiencies are generally understood, the focus of SOFIE extinctions is PMCs and improvements directed at stratospheric aerosol measurements are of a lower priority.

[1]The tropopause altitude at SOFIE latitudes is ~9 km. PMC are detected at altitudes of roughly 80 - 92 km.
[2]Validation papers are listed on the SOFIE website (sofie.gats-inc.com) under "Publications." Please contact Mark Hervig (m.e.hervig@gats-inc.com) if you would like an electronic copy of any of these documents.
[3]The Southern Hemisphere (SH) is measured by SOFIE sunrise events, and the Northern Hemisphere (NH) by sunsets.

Table 2. SOFIE Version 1.3 Level 1 Data Description*

Band (wavelength)	Product	Exoatmospheric Altitude (km)	Sunrise Signal Correction	Sunset Signal Correction
1 (0.292 μm)	O_2 strong	105 km	HOC	HOC
2 (0.330 μm)	O_2 weak	105 km	HOC	HOC
3 (0.867 μm)	PMC strong	95 km	HOC	HOC
4 (1.037 μm)	PMC weak	95 km	HOC	HOC
5 (2.462 μm)	H_2O weak	95 km	HOC	HOC
6 (2.618 μm)	H_2O strong	95 km	HOC	HOC
7 (2.785 μm)	CO_2 strong	120 km	HOC	HOC
8 (2.939 μm)	CO_2 weak	120 km	HOC	HOC
9 (3.064 μm)	PMC strong	95 km	HOC	HOC
10 (3.168 μm)	PMC weak	95 km	HOC	HOC
11 (3.384 μm)	CH_4 strong	90 km	HOC	HOC
12 (3.479 μm)	CH_4 weak	90 km	HOC	HOC
13 (4.324 μm)	CO_2 strong	145 km	Linear	Linear
14 (4.645 μm)	CO_2 weak	145 km	HOC	HOC
15 (5.006 μm)	NO weak	160 km	HOC	HOC
16 (5.316 μm)	NO strong	160 km	Gomez et. al.	Gomez et. al.

*SOFIE uses three different methods for correcting signal drift related to heating during solar view. The exoatmospheric height is where the signals are normalized to determine transmission. This represents the upper limit in altitude for retrievals, although retrievals may not extend this high.