High Resolution Reference Solar Spectrum for TEMPO/GEMS and beyond

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Reference Solar Spectra

- No absolutely calibrated solar reference spectrum from single source due to limitations
 - Differs depending on the sources of data (sampling, resolution, SRF and accuracy)
- High resolution reference solar spectrum is important for the calibration of the hyperspectral instrument such as TEMPO and GEMS
- As the calibration is sensitive to the choice of high resolution solar reference, we would like to improve over existing high resolution reference spectra



Reference Solar Spectra

- Reference solar spectra available for TEMPO/GEMS
 - Considering the radiometric, spectral accuracy, spectral sampling and resolution for TEMPO & GEMS (high-resolution spectrometer)
 - ✓ Few high-resolution reference spectra are available

	Spectrum	Wavelength range [nm]	Spectral resolution [nm]	Spectral sampling [nm]	Uncertainty [%]	references
Low	NRLSSI2	115.50-99999.50	1.00	1.00	2-4	Coddington <i>et al</i> . (2015)
resolution references High resolution references	ATLAS	120.00-2400.00	0.25-0.50	0.05-0.60	2-4 for 120-2400 nm	Thuillier <i>et al</i> . (2004)
	WHI	0.10-2400.00	1.00-30.00	0.01	2-4 for 116-2400 nm	Woods <i>et al</i> . (2008)
	KNMI	235.00-520.00	0.025	0.01	<4 for 300-500 nm	Dobber <i>et al</i> . (2008)
	SAO2010	200.07-1000.99	0.04	0.01	< 5 for 300 -1000 nm	Chance and Kurucz (2010)
	Ftsc SAO	293.00-1626.57		0.003		Chance and Kurucz (2010)
	JPL (transmittance)	380.00-2400.00		0.00014		Toon (2014)

Table. Examples of currently available reference solar spectra and their characteristics

Reference Solar Spectra

- JPL transmittance
 - Newly derived solar linelist
 - Very high resolution (0.01 cm⁻¹) with broad wavelength range (600-26316 cm⁻¹, 2400 -378 nm)
 - not radiometrically calibrated





Spectral Calibration

• Sensitivity tests for GEMS wavelength calibration



Figure . Flow chart of spectral calibration algorithm for GEMS

- Tested for the GEMS ozone retrieval range (300 to 340 nm)
- Input perturbation

Shift	Squeeze	FWHM	
1 (%)	0.5 (%)	+0.1 (nm)	

- Considered spectral parameters
 - ✓ Reference solar spectrum
 - ✓ SRF
 - ✓ SNR
- Check the algorithm performance due to uncertainty of spectral parameter

Spectral Calibration

• What if we use a different reference spectrum?



Algorithm input				Algorithm output				
Shift	Squeeze	FWHM	Ref. Solar spectrum	Ref. True Solar solar bectrum spectrum		Squeeze	FWHM	Chi square
-0.0100	0.0050	0.7000	SAO2010	SAO2010	-0.0102	0.0050	0.6987	5.456e ⁻⁶
-0.0100	0.0050	0.7000	KNMI	KNMI	-0.0102	0.0050	0.6989	4.887e⁻ ⁶
-0.0100	0.0050	0.7000	SAO2010	KNMI	-0.0132	0.0050	0.6988	2.563e ⁻⁴
-0.0100	0.0050	0.7000	KNMI	SAO2010	-0.0068	0.0050	0.7018	2.751e ⁻⁴

Spectral Calibration

- Sensitivity tests results
 - It is highly sensitive to the reference solar spectrum
 - \checkmark Due to the uncertainty of reference solar spectrum,
 - Calibration performance could be considered as lower than actual performance
 - The derived shifts could be different from actual wavelength variability
 - \checkmark Minimum chi-square value increases more than an order

Algori	thm Input	Algorithm Output		
ReferenceAssumedspectrummeasurement		X² (e⁻⁵)	ΔR (%)	
KNMI	KNMI	4.89	0.012	
SAO2010	SAO2010	5.46	0.014	
KNMI	SAO2010	275	0.077	

(ΔR is mean differences of radiance)

Current References

- SAO2010 vs. KNMI reference spectrum
 - There are non-negligible differences between the two at TEMPO/GEMS resolution (FWHM = 0.6 nm)



Differences between SAO2010 and KNMI (FWHM= 0.6 nm)

Comparison between SAO2010 and KNMI at initial resolution and lower resolution (FWHM= 0.6 nm)

Current References

- SAO2010 vs. KNMI reference spectrum
 - Differences between two are mainly caused by using of the different data sources



Requirements for Update

- Preparation of reference spectrum for TEMPO/GEMS
 - TEMPO/GEMS top-level requirement

	ΤΕΜΡΟ	GEMS
Observational Range [nm]	290 -740	300 - 500
Spectral Sampling [nm]	0.2	0.2
Spectral Resolution [FWHM, nm]	0.6	0.6

- Reference solar spectrum requirement
 - ✓ Absolute radiometric accuracy < 3-4% (Dobber et al.,2008)
 - ✓ Original spectral resolution > TEMPO/GEMS resolution
 - ✓ Fully *Nyquist* sampled (Chance et al.,2010)

SAO2010 and JPL (over 380 nm) are only great references for TEMPO&GEMS and beyond after calibration with low resolution (WHI below 310 nm & ATLAS over 310 nm)!!

Method

• Updating SAO2010/JPL

- Fitting the SAO2010/JPL with reference (WHI/ATLAS) to obtain SRF of reference & scaling factors; same spectral feature
- 2 Convolution of the SAO2010/JPL spectrum with the derived function ;same spectral resolution
- ③ Calculating the ratio between convolved spectrum with reference (R)
- Obtaining the new convolved SAO2010/JPL applied ratio (R') to SAO2010/JPL;

new convolved SAO2010/JPL

= convolved SAO2010/JPL * R



Figure. Process for updating SAO2010

Method

• Deriving the SRF of references based on Super-Gaussian function (Beirle et al., 2016)

1. Spectral fitting (OE method)
$$I_{ref} = \frac{\int I_{SAO}\phi_{ref}d\lambda}{\int \phi_{ref}d\lambda} \times scaling factors$$

$$S(x) = \frac{k}{2\varpi\Gamma(1/k)} e^{-\left|\frac{x}{\omega}\right|^{k}}$$

 ϖ is for the width k is for the shape of S





A significant improvement in the shorter wavelength range is evident



Updated SAO spectrum

Comparison between before and after update (= $\frac{updated SAO2010-SAO2010}{updated SAO2010} * 100(\%)$)

- Comparison new SAO2010 with other reference solar spectra
 - Increased consistency among the spectra with the decreased mean radiometric differences

Reference Spectrum	Correlation Coefficient	Mean Radiometric Differences [%]	
SAO2010/NRLSSI2	0.9659	1.7275	
SAO2010/ATLAS3	0.9738	0.3223	
SAO2010/KNMI	0.9464	1.6985	
NewSAO2010/NRLSSI2	0.9754	1.4045	
NewSAO2010/ATLAS3	0.9899	0.0854	
New SAO2010/KNMI	0.9689	1.0593	

Comparison among reference spectra for 300 -500 nm range at FWHM 1.0 nm

Calibrated JPL



 We would compare calibrated JPL with SAO2010 within oxygen air band A & B to figure out which is better

Discussion and Further Study

- Radiometric calibrated high resolution reference solar spectra (SAO2010 & JPL spectra) have been derived based on low resolution reference spectra (WHI & ATLAS) with Super-Gaussian function
- Additional optimization and detailed analysis among reference solar spectra is in progress
- We will derive high resolution solar reference spectra from 200-2400 nm at various spectral resolution (e.g., 0.01 nm, 0.01 cm⁻¹)

Thank You

Reference Solar Spectra



• Updating SAO2010



Whole Heliosphere Interval (WHI) (Mar-Apr 2008)

- obtained from simultaneous observation during solar cycle minimum conditions
- 0.1-6 nm: XPS-TIMED
 - Thermosphere, Ionosphere, Mesosphere, Energetics, and Dynamics
 - XUV (X-ray UV) Photometer System (XPS)
 - ✓ 0.1-nm resolution from spectral model fitted to 7-nm broad band XPS measurement
- 6-105 nm: MEGS (rocket)-EVE
 - Multiple EUV Grating Spectrograph
 - EUV Variability Experiment (EVE)
 - ✓ 0.1-nm spectral resolution measurement binned down to 0.1-nm intervals higher resolution spectrum (0.01-0.025 nm intervals) also available rocket launched on 14-Apr-08
- 105-116 nm: SEE-TIMED
 - Solar EUV Experiment (SEE)
 - ✓ 0.1-nm intervals, but 0.4-nm spectral resolution
- 116-310 nm: SOLSTICE-SORCE
 - Solar Radiation and Climate Experiment (SORCE)
 - Solar Stellar Irradiance Comparison Experiment
 - ✓ .1-nm spectral resolution measurement binned down to 0.1-nm intervals
- 310-2400 nm: SIM-SORCE
 - Spectral Irradiance Monitor
 - ✓ low-resolution prism measurement is interpolated to 0.1-nm intervals
 - ✓ SIM resolution is about 1 nm at 300 nm and about 34 nm at 1200 nm

Thuillier et al 2004

- widely used for the low resolution solar reference
- 0.5-120 nm: Rocket
- 120-200 nm: SUSIM-UARS/SOLSTICE-UARS
- 200-400 nm
 - SUSIM-UARS/SOLSTICE-UARS/
 - SUSIM-ATLAS1-3/SSBUV-ATLAS1/
 - SOLSPEC-ATLAS1-3/SOLSTICE-ATLAS1-3
- 400-870 nm: SOLSEPC-ATLAS1-3
- 870-2400 nm: SOSP-EURECA

 An empirical solar linelist has been generated by simultaneous fitting of ATMOS, MkIV, Kitt Peak, Denver U, and TCCON spectra. The telluric absorptions were fitted using the HITRAN linelist and any remaining, airmass-independent absorptions were attributed to the sun. Together with a simple lineshape function, this linelist allows the computation of a solar pseudotransmittance spectra, for disk-center, diskintegrated, or intermediate cases. These spectra have been validated using MkIV, Kitt Peak, ACE, and GOSAT spectra.

- SAO 96
 - 230-800 nm, 0.01 nm resolution/0.02 FWHM
 - Based on ground-based measurements (Kurucz 1984)
 & balloon measurements (Hall and Anderson 1991)
 - ✓ Converted to vacuum wavelengths.
 - ✓ Ground data was recalibrated using 4 O2 lines (accuracy of better than 0.001 nm)
 - ✓ Balloon data were recalibrated in wavelength using 20 selected atomic reference lines. (accuracy of 0.003 nm)
 - ✓ Spectra were resampled at even 0.01 nm increments, employing a triangular filter of 0.02 nm FWHM and linearly merged over the 300-305 nm

Spectru m	Wavelength/Sampling (nm)	Resolution (nm)	Resolution (nm) Sources	
Kitt Peak	293.09-1627.02 vacuum nm derived from the Fourier transform spectroscopy measurements of the Sun 0.0003 – 0.001	0.0005	Kurucz R. L., I. Furenlid, J. Brault, and L. Testerman, <i>Solar</i> <i>Flux Atlas from 296 to 1300 nm</i> (National Solar Observatory, Sunspot, New Mexico, 1984) 240 pp. http://kurucz.harvard.edu/sun.html	
Hall and Anderson	200-310 0.01 measured near 40 km in the stratosphere in 1978 and 1983, have been combined and extrapolated to zero optical depth to provide a reference spectrum in 0.1-Å	0.025	Hall L. A. and G. P. Anderson (1991), High-resolution solar spectrum between 200 and 3100 Å," <i>J.</i> <i>Geophys. Res.</i> 96, 12, 927–12,931	within 0.04 Å.

- SAO produce the calibrated solar spectrum (235-1100 nm) as part of OMPS instrument and algorithm development
 - SOLSTICE and SUSIM (Woods et al., 1996)+ LOWTRAN/MODTRAN
 - Linearly merged 405.6-410.6 nm
- OMI spectrum (Dobber et al., 2006)
 - Kitt peak (Kurucz 1984) and Hall & Anderson 1991
 - Use combined low resolution spectra
 - ✓ SUSIM from UARS (Floyed et al., 2003) up to 410 nm, 0.15 nm resolution
 - Triangular slit
 - ✓ Balloon spectrum for SCIAMACHY validation (Gurlit et al., 2005) from 400 nm
 - Square shaped slit function

- SAO 2010
 - Use updated kitt peak (agreement with Thuillier et al., ; better than 1% at 20 nm spectral resolution)
 - ✓ Large scale features by O3, O2-O2 were computed and divided out.
 - ✓ The computed line spectrum were adjusted for an match to the observed spectra
 - ✓ Artifacts from wavelength mismatches, deep lines, etc, were removed by hand.
 - Updated kitt peak data and H&A spectra are each convolved to a Gaussian FWHM of 0.04 nm and sampled to 0.01 nm
 - Linearly merged to 300 to 305 nm

Compare SAO 2010 & OMI

	Range (nm)	Sampling (nm)	Resolution (nm)	High resolution	Low resolution	issues
SAO 2010	200.07- 1000.99	0.01	0.04	Kitt peak (2005) Hall & Anderson		Radiometric calibration
ОМІ	250-550	0.01	0.025	Kitt peak (1984) Hall & Anderson (SAO 96)	SUSIM (~410 nm) (Floyd et al 2003) Balloon (400 nm ~) (Gurlit et al 2005)	Under- sampling
Updated SAO	200.07- 1000.99	0.01	0.04	SAO 2010	WHI (~310 nm) (Woods et al 2009) ATLAS1&3 (300 nm~) (Thuillier et al 2004)	

- Allow overlapping between adjacent windows.
 - For example, if each window is 10 nm, then fit
 292-302 nm, 300-310 nm, 308-318 nm and only
 apply the results to non-overlapped regions, i.e.,
 results from fitting 300-310 nm to 302-308 nm.





Current References



Current References

