Trace gas training set for TES
Updated November 2010 by Yaping Xiao

The list of molecules in OSS with order number:
1: H2O 2: CO2 3: O3 4: N2O 5: CO 6: CH4 7: O2 8: NO
9: SO2 10: NO2 11: NH3 12: HNO3 13: OH 14: HF 15: HCL 16: HBR
17: HI 18: CLO 19: OCS 20: H2CO 21: HOCL 22: N2 23: HCN 24: CH3CL
25: H2O2 26: C2H2 27: C2H6 28: PH3 29: COF2 30: SF6 31: H2S 32: HCOOH
33: HO2 34: O 35:CLONO2 36: NO+ 37: HOBR 38: C2H4 39: CH3OH
51: CCl4 52: CF4 54: F11 56: F12 58: F22

As of October 2010, we update

O3,CH4,N2O, CO, F11(CFCl3), F12(CF2Cl2), HNO3	GMI daily profiles in 2006
CCl4	GMI monthly profiles in 2006
OCS	AER 2D model
NH3, HCOOH, CH3OH, C2H2, C2H4, HCN	GEOS-Chem monthly profiles
CO2, SO2, CF4, F22 (CHClF2)	no update

Table 1. Fixed Gases.

O2	AFGL Standard Atmosphere
NO	AFGL US Standard Atmosphere
NO2	AFGL US Standard Atmosphere
N2	AFGL Standard Atmosphere

O2 is not an issue in this spectral region and could have been omitted.
NO, and NO2 and very minor species that won't likely be seen in the nadir spectra.

Table 2. Old versus New OSS files

* The reason we choose 182 profiles in the new OSS file is to accommodate both the number of samples in the original ECMWF data sets (52 profiles) used for the OSS training, and the number of OCS profiles available (228 profiles). Thus the new training set has 52*7 / 2 = 182 profiles, versus the 364 (=52*7) profiles in the old training set.

old OSS file	new OSS file
364 profiles, randomized	182 profiles *
20 species	15 species updated except H2O, CO2, SO2, CF4, F22
/project_static/p1411/oss4TES/minor_spieces/ecmwf52x7_101_vTES_em_0.7-1.0.dat	/data_static/carbon/GMI/gmi_2oss.dat
unit g/g	unit g/g
Reading program: /data_static/carbon/GMI/read_oss_var.pro	Writing program: /data_static/carbon/GMI/write_oss_var.pro

Line 2-18: 101 pressure levels
Line 20-21: HITRAN numbers in order(the oss order number in parenthesis)
Only for those line 21 value is equal to 0
1:H2O (1) 2:CO2 (2) 3:O3(3) 4:N2O(4) 5:CO(5) 6:CH4 (6) 7:SO2(9)
8:NH3 (11) 9:HNO3 (12) 10:OCS(19) 11:HCN(23) 12:C2H2(26) 13:HCOOH (32)
14: C2H4 (38) 15:CH3OH (39) 16:CCl4 (51) 17:CF4 (52) 18: F11(54)

19: F12 (56) 20: F22 (58) Line 27-43: temperature profile (101 values) Line 44: Tskin (1 value) ……Then the profiles for the species as specified on line 20-21.	
some original profiles where the old oss file has based on: */project_static/p1411/oss4TES/minor_spieces/* C2H2_vmr_MIPAS.txt C2H4_vmr_UARS.txt CH3OH_vmr_geos_chem_mean.txt HCN_vmr_MIPAS.txt HCOOH_vmr_UARS.txt NH3_vmr_bg.txt F22_vmr_MIPAS.txt	

Table 3: Variable Gases

GMI daily profiles with the full selection and original vertical grids (~40GB) are saved
`/data_static/carbon/GMI/gmic_G5aura_2006_xxx.idaily.nc`
`/data_static/carbon/GMI/gmi_species_fixed.daily.[O3,CH4,N2O, CO, CFC13, CF2C12, HNO3].sav` (IDL save format)

GMI monthly profiles of CCl4:
`/data_static/carbon/GMI/gmic_G5aura_2006_MMM.amonthly.nc`
`/data_static/carbon/GMI/gmi_species_fixed.monthly.CCl4.sav`

The selected profiles are archived under
`/data_vs/data_static/carbon/GMI/oss_output_txt/`

	Old version	New Version	Other possible sources	comments
H2O	ECMWF with noise added; same as standard training set	ECMWF with noise added; same as standard training set		
O3	ECMWF with noise added; same as standard training set	GMI Daily profiles in 2006	GEOS-Chem MOZART	Compared to GC and MOZART, GMI gives wider altitudinal coverage
CO2	GMI ±10°lat, ±1 month match, plus secular trend, noise added on primary and secondary levels and interpolated	No update	GEOS-Chem	Old version shows more variability than GEOS-Chem
CH4	GMI ±10°lat, ±1 month match, plus secular trend, noise added on primary and secondary levels and interpolated	GMI Daily profiles in 2006	GEOS-Chem MOZART	Compared to GC and MOZART, GMI gives wider altitudinal coverage
N2O	GMI ±10°lat, ±1 month match, noise added on primary and secondary levels and interpolated	GMI Daily profiles in 2006	MOZART HIPPO	GMI has wider altitudinal coverage
CO	GMI ±10°lat, ±1 month match, noise added on primary and secondary levels and interpolated	GMI Daily profiles in 2006	GEOS-Chem MOZART	GMI has wider altitudinal coverage
F11	GMI ±10°lat, ±1 month match, noise added on primary and secondary levels and interpolated	GMI Daily profiles in 2006		Only available from GMI, also some information from Satellite retrieval [²Hoffmann et al 2008]