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ATMOSPHERE CONSTITUENTS SPECTRA MODELING UP TO 25 KM ALTITUDE

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Abstract

Measurement of atmosphere constituents altitude distribution is important component of atmosphere monitoring (atmosphere physics and chemistry, global warming, etc.). Central aerological observatory of Russia has airplane-laboratory M55 (22 km altitude) [1]. Due to Russian state program airplane-laboratory based on Jak-42d (9.1 km altitude) is under development [2]. GPI is developing TDLS based complexes to measure H_2O, CO_2, CO, CH_4 concentration [3].
To select analytical spectral lines and to optimize the complexes operation modeling of atmosphere constituents spectra up to 25 km altitude is necessary subject of present paper. Software “line-by-line” was developed to model atmosphere constituents’ spectra. Software developed is using molecular spectral data from HITRAN 2008 [4] as well as atmosphere models available. Using software developed several atmosphere constituents (, etc.) spectra altitude dependences were modeled.

[1] http://www.aviaport.ru/directory/aviation/m55
[2] http://www.aviaport.ru/directory/aviation/jak42d/
[3] V.Galaktionov, V.Khattatov, A.Nadezhdinskii, Ya.Ponurovskiy, D.Stavrovskii, I.Vyazov, V.Zaslavskii , TDLS complex development for airplane-laboratory “Atmosphere”, p.44. ABSTRACTS OF PAPERS 7th International Conference on Tunable Diode Laser Spectroscopy, July 13-17, 2009 Zermatt, Switzerland
[4] http://cfa-www.harvard.edu/HITRAN

Airplane - laboratories

M-55	
Speed	740 km/h
Distance	1350 km
Altitude	22 km

Central aerological observatory of Russia has in operation airplane-laboratory M55.

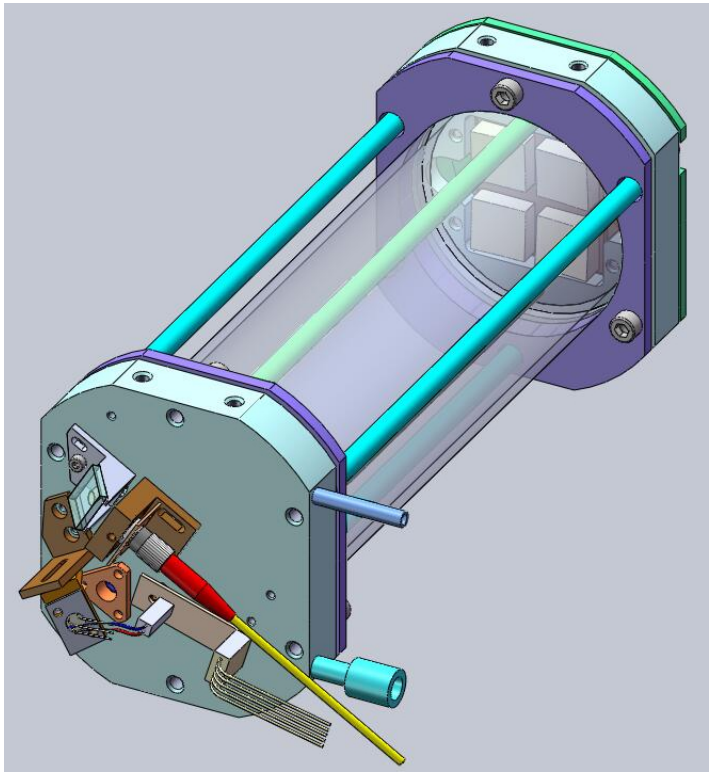
Jak-42d	
Speed	730 km/h
Distance	4100 km
Altitude	9.1 km

Due to Russian state program airplane-laboratory based on Jak-42d (9.1 km altitude) is under development.

The complex operation parameters

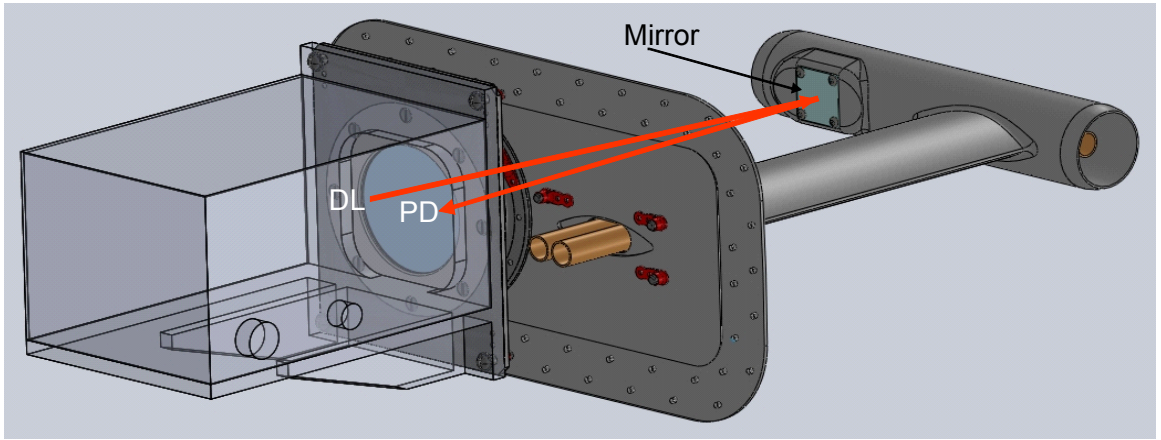
Following molecules were selected for detection.

Molecule	Concentration variation, ppm
H_2O	3-15000
CO_2	363-365
CH_4	1.6-1.8
CO	0.05-0.12



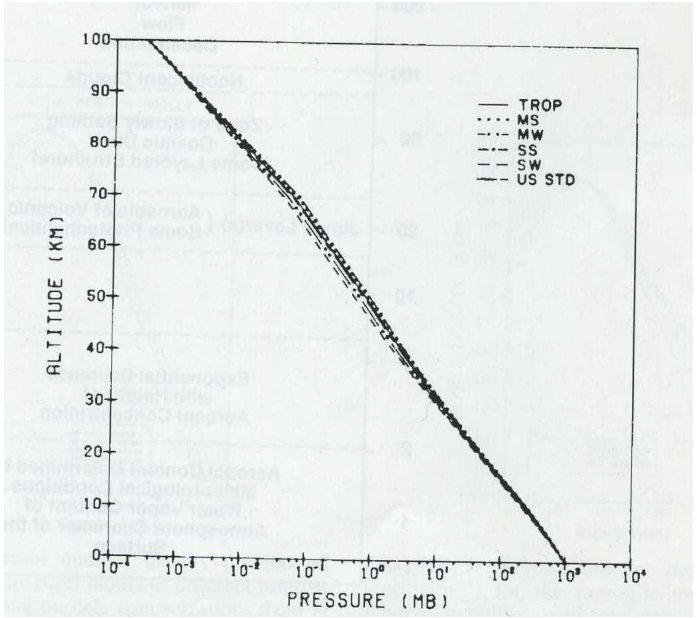
"Chernin" matrix optical system (left) is using to measure molecules concentration. Parameters: P = 100 mBar, T – room temperature, L = 40 m.

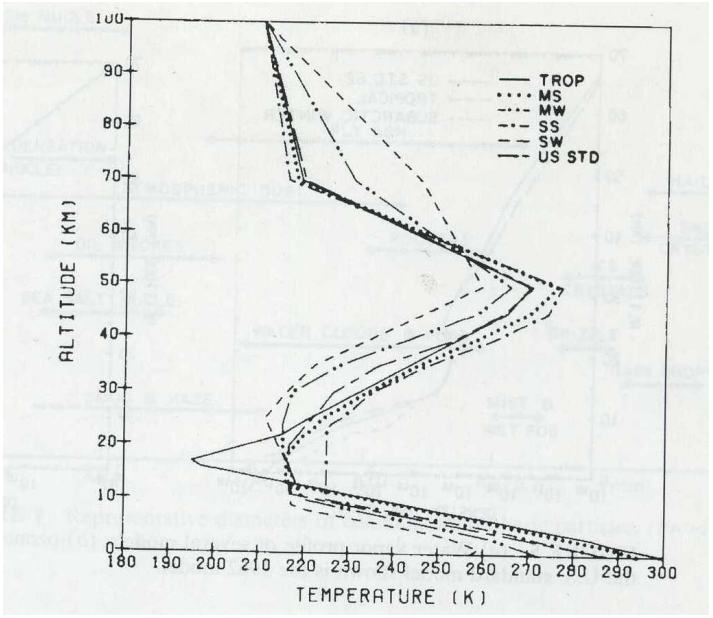
The complex water channel contains additional module to measure atmosphere turbulence (right). Parameters: P and T are atmosphere pressure and temperature, respectively, L = 40 cm.

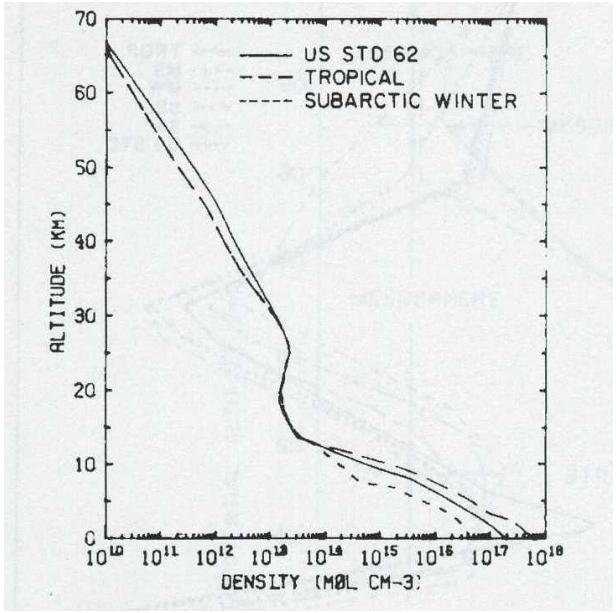


Atmosphere models

Six atmosphere models were considered.







Pressure (left), temperature (mid), and humidity (right) vs. altitude for six model atmospheres: tropical (TROP), midlatitude summer (MS), midlatitude winter (MW), subarctic winter (SW), and US standard (US STD).
For majority of modeling US standard atmosphere model was used.

Spectra modeling

Spectra modeling was based on HITRAN 2008 spectral database [1], atmosphere models considered in previous slide, and software “LINE-by-LINE” developed [2].

Example of 160-character HITRAN line-transition format.

FORTRAN Format (I2,I1,F12.6,1P2E10.3,0P2F5.4,F10.4,F4.2,F8.6,2A15,2A15,6I1,6I2,A1,2F7.1) corresponding to:					
Mol	I2	Molecule number	δ_{air}	F8.6	Air-broadened pressure shift of line transition in cm^{-1}/atm @ 296K
Iso	I1	Isotopologue number (1= most abundant, 2= second most abundant, etc.)	v′, v″	2A15	Upper-state global quanta, lower-state global quanta
ν_{ij}	F12.6	Wavenumber in cm^{-1}	q′, q″	2A15	Upper-state local quanta, lower-state local quanta
S_{ij}	E10.3	Intensity in cm^{-1}/(molecule x cm^{-2}) @ 296K	ierr	6I1	Uncertainty indices for wavenumber, intensity, air- and self-broadened half-widths, temperature-dependence, and pressure shift
A_{ij}	E10.3	Einstein-A coefficient	iref	6I2	Indices for table of references corresponding to wavenumber, intensity, air- and self-broadened half-widths, temeperature-dependence, and pressure shift
γ_{air}	F5.4	Air-broadened half-width (HWHM) in cm^{-1}/atm @ 296K	Flag	A1	Flag (*) for lines supplied with line-coupling algorithm
γ_{self}	F5.4	Self-broadened half-width (HWHM) in cm^{-1}/atm @ 296K	g′	F7.1	Upper-state statistical weight
E″	F10.4	Lower state energy in cm^{-1}	g″	F7.1	Lower-state statistical weight
n_{air}	F4.2	Coefficient of temperature dependence of air-broadened half-width			

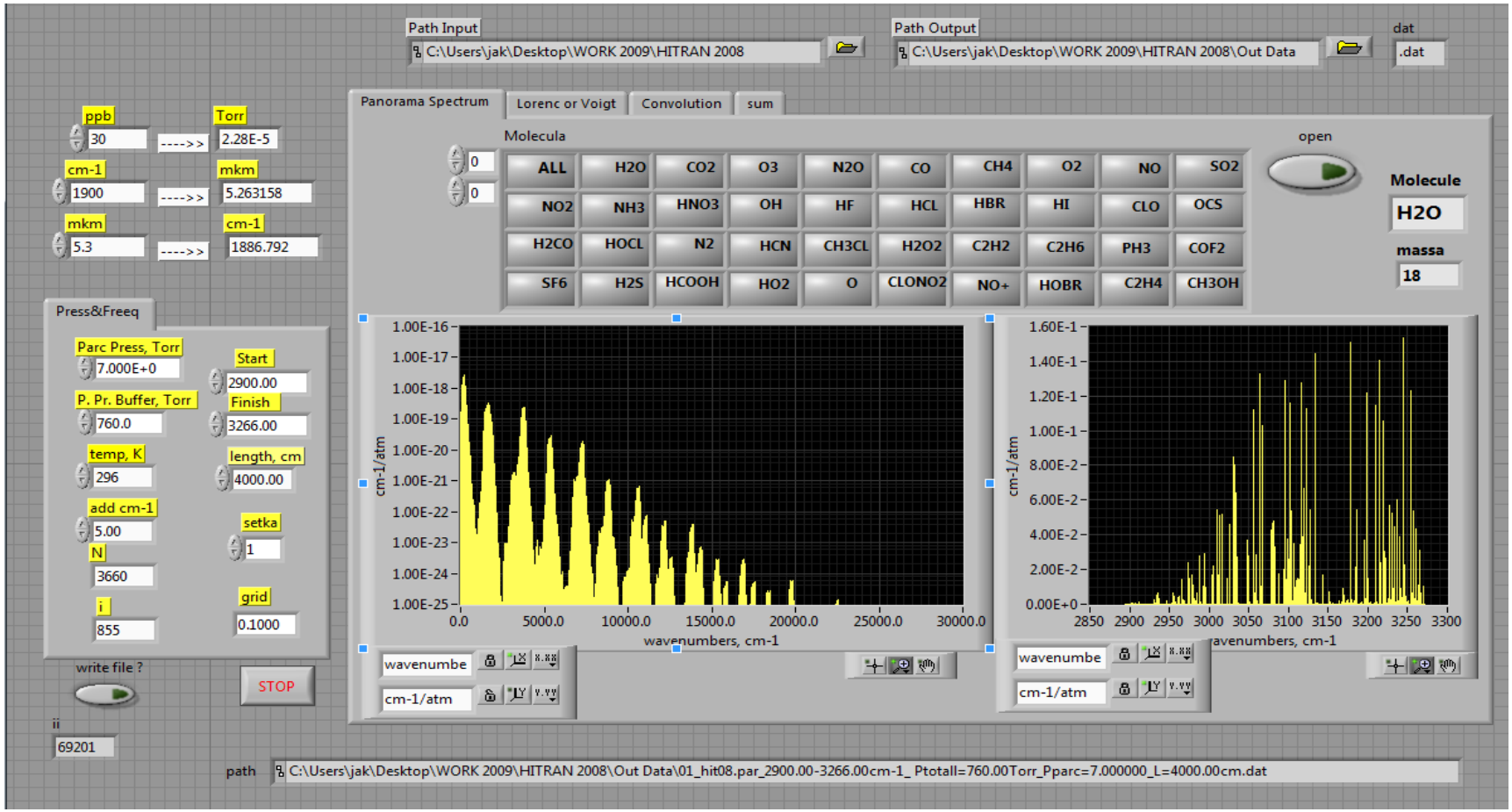
HITRAN Molecule Number	Molecule Chemical Symbol	Number of trans-itions	HITRAN Molecule Number	Molecule Chemical Symbol	Number of trans-itions
1	H_2O	63197	21	HOCl	16276
2	CO_2	62913	22	N_2	120
3	O_3	311481	23	HCN	4253
4	N_2O	47835	24	CH_3Cl	31119
5	CO	4477	25	H_2O_2	100781
6	CH_4	251440	26	C_2H_2	3517
7	O_2	6428	27	C_2H_6	4749
8	NO	102280	28	PH_3	11790
9	SO_2	38853	29	COF_2	70601
10	NO_2	104223	30	SF_6	22901
11	NH_3	29084	31	H_2S	20788
12	HNO_3	271166	32	HCOOH	24808
13	OH	42373	33	HO_2	38804
14	HF	107	34	O	2
15	HCl	613	35	$ClONO_2$	32199
16	HBr	1293	36	NO^+	1206
17	HI	806	37	HOBr	4358
18	ClO	7230	38	C_2H_4	12978
19	OCS	19920	39	CH_3OH	19899
20	H_2CO	2702			

Parameters of HITRAN 2008 spectral database.

[1] http://www.cfa.harvard.edu/HITRAN/

[2] A.Nadezhdinskii, Ya.Ponurovskiy, “LINE-by-LINE” SOFTWARE FOR SPECTRA SIMULATION ”, p.59. ABSTRACTS OF PAPERS 7th International Conference on Tunable Diode Laser Spectroscopy, July 13-17, 2009 Zermatt, Switzerland

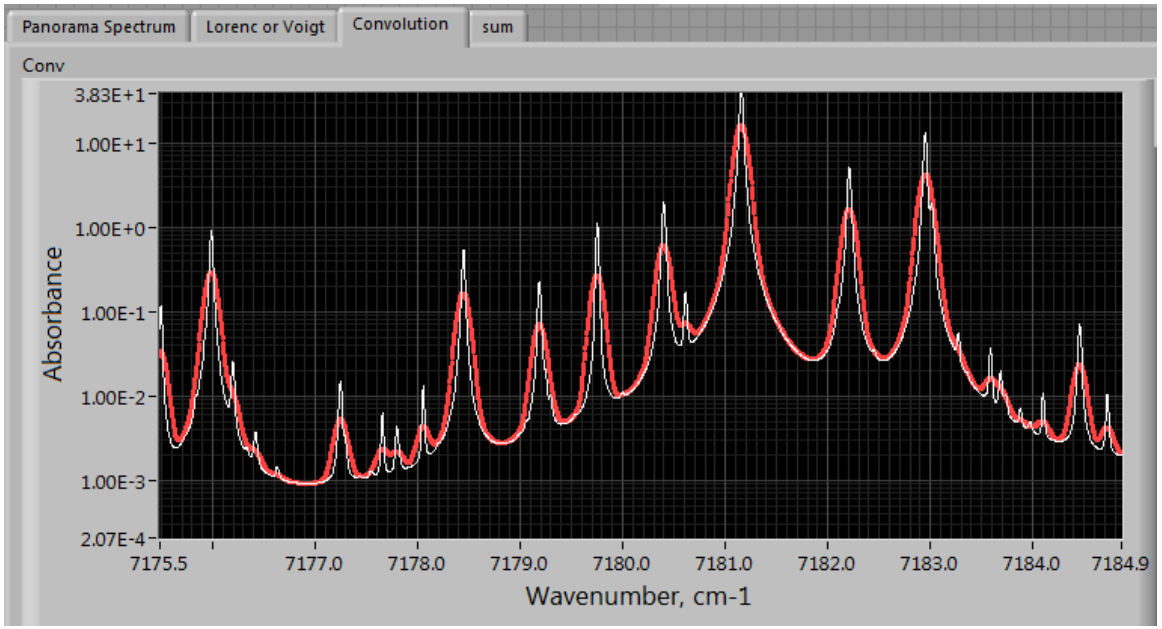
“LINE-by-LINE” software



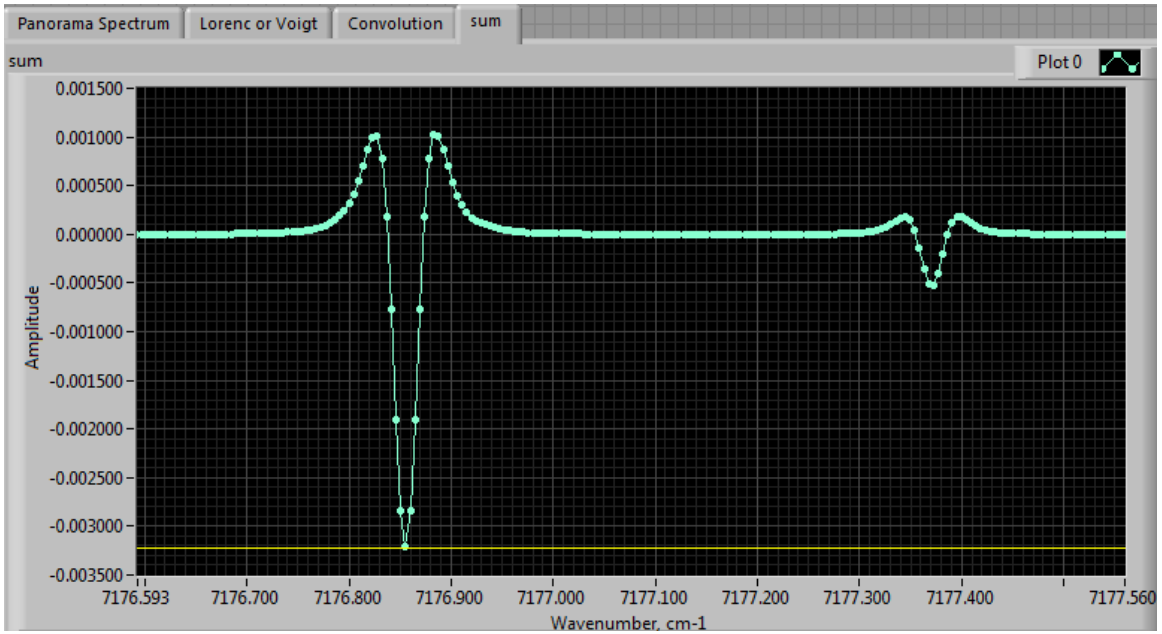
User can select molecule from HITRAN 2008, can determine experimental parameters: total and partial pressures, temperature, optical length, and spectral range. The software performs convolution of model spectrum with spectral line shape. In present case water vapor spectrum modeling is presented.

“LINE-by-LINE” can analyze spectra of 4 different molecules.

“LINE-by-LINE” additional options



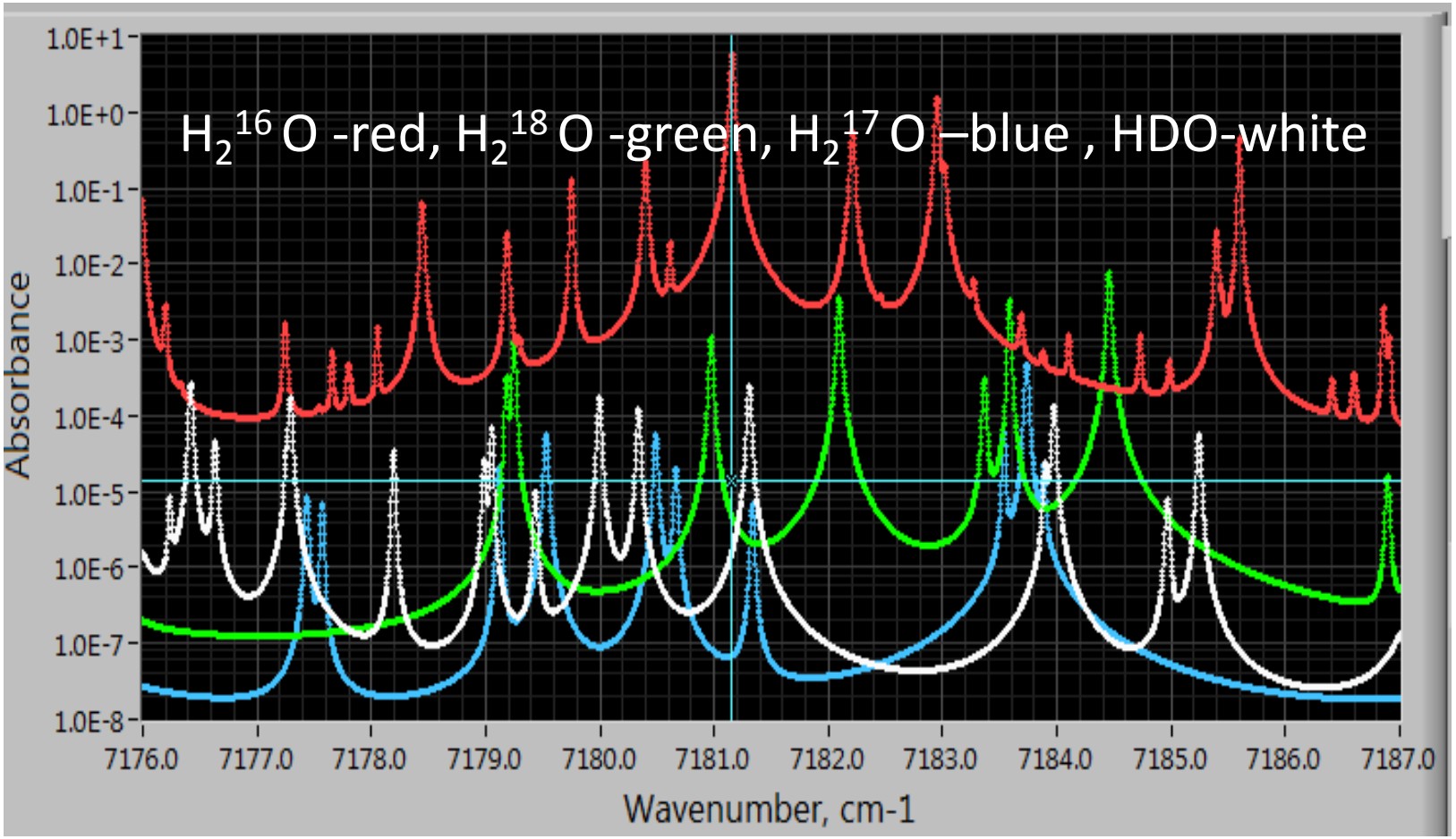
Water vapor spectrum (white) convolution with Gaussian function with HWHH 0.06 cm^{-1} (red).



Water vapor absorbance second derivative.

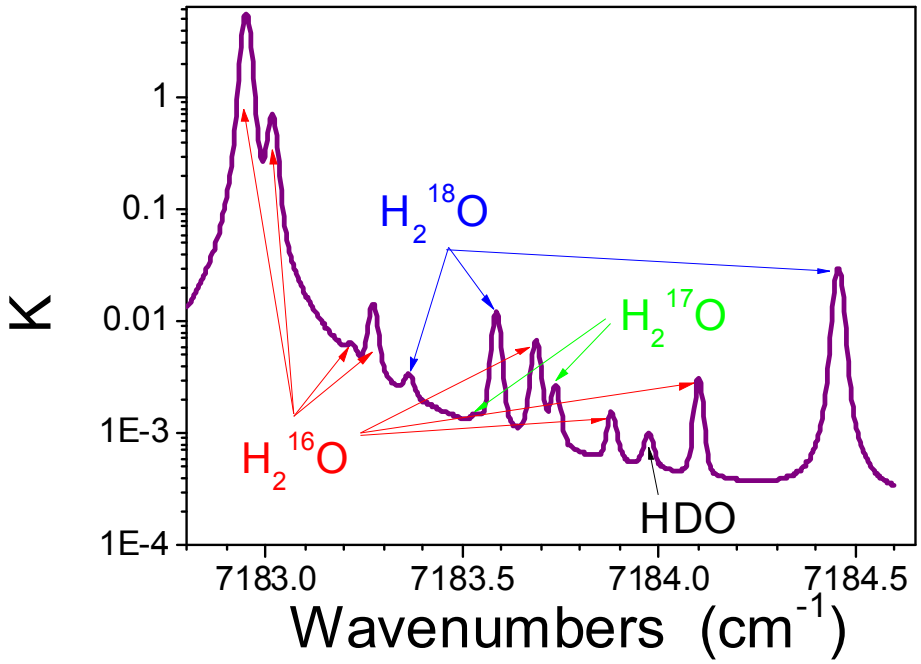
Water channel

Tasks of water vapor channel: humidity and isotopes ratio measurements inside “Chernin” matrix optical system, humidity and turbulence measurements outside of airplane. Spectral range near 1.39 μ was selected as analytical one.

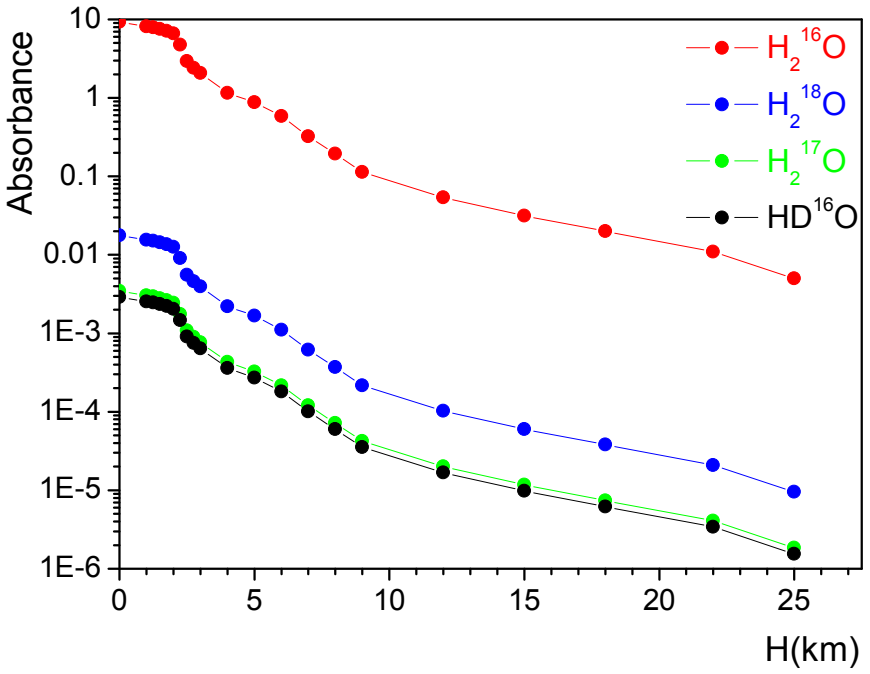


Model water vapor spectra for following parameters: L=40m, P=100mBar, C=1700ppm

Humidity and isotopes measurements in “Chernin” matrix optical system



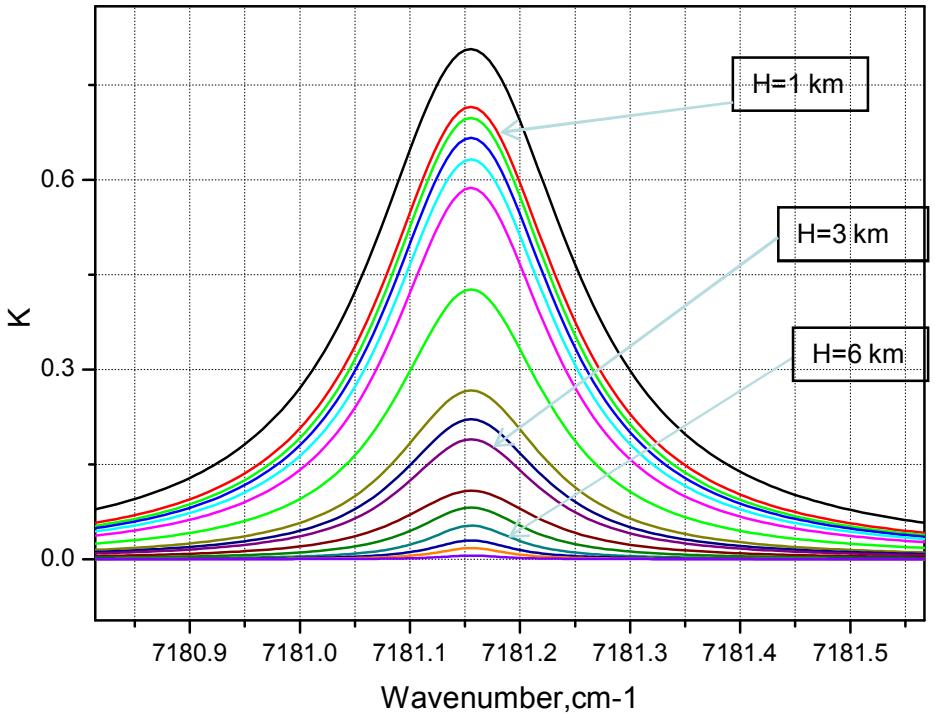
Model water vapor spectrum and lines identification.
Parameters: L = 40 m, P = 100 mBar, natural abundance.



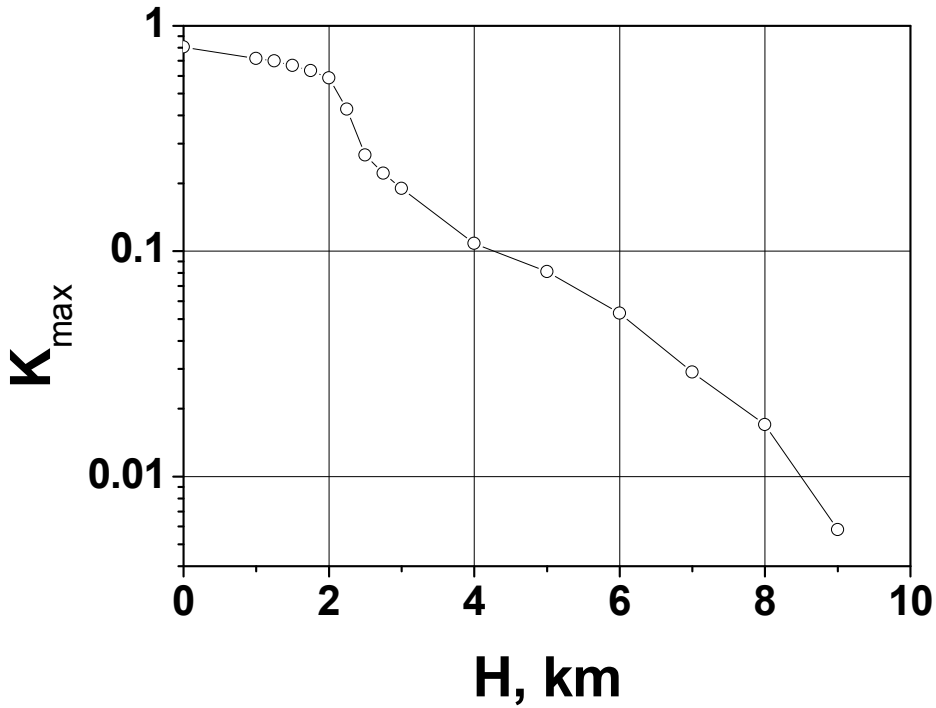
Altitude dependence of maximum line absorbance for different water atoms isotopes.

Conclusion: Different isotopes can be detected up to 25 km altitude.

Humidity and turbulence measurements in open atmosphere



Analytical line absorbance modeling for different altitudes.
Parameters: L = 40 cm.
US standard atmosphere was used.



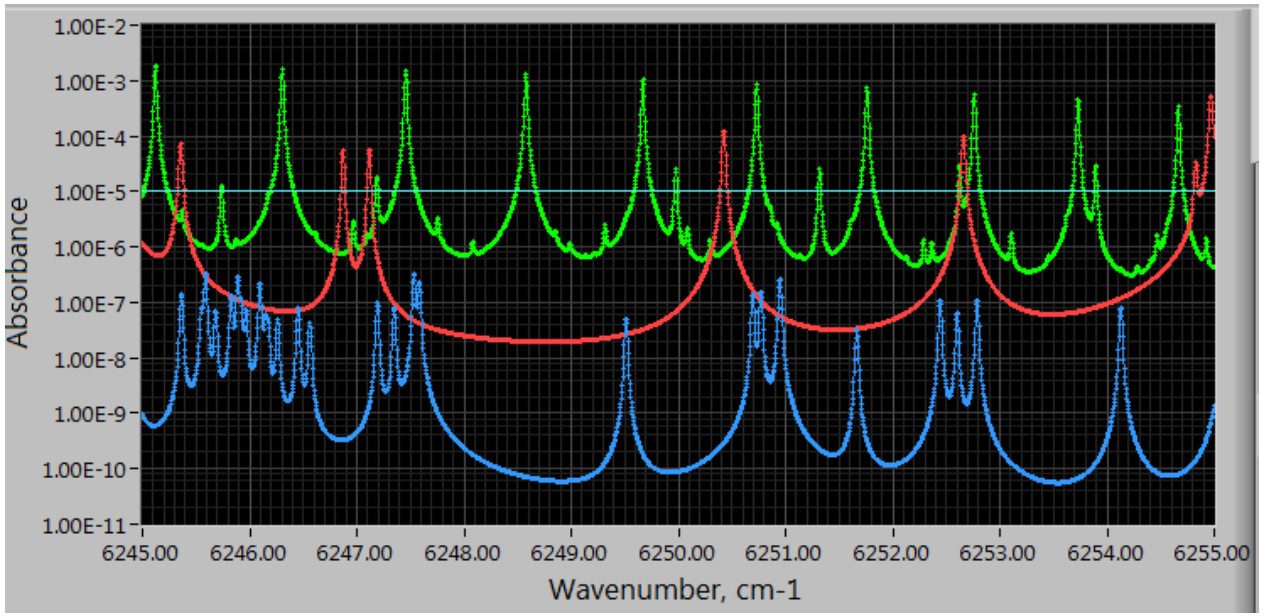
Maximum absorbance as function of altitude.

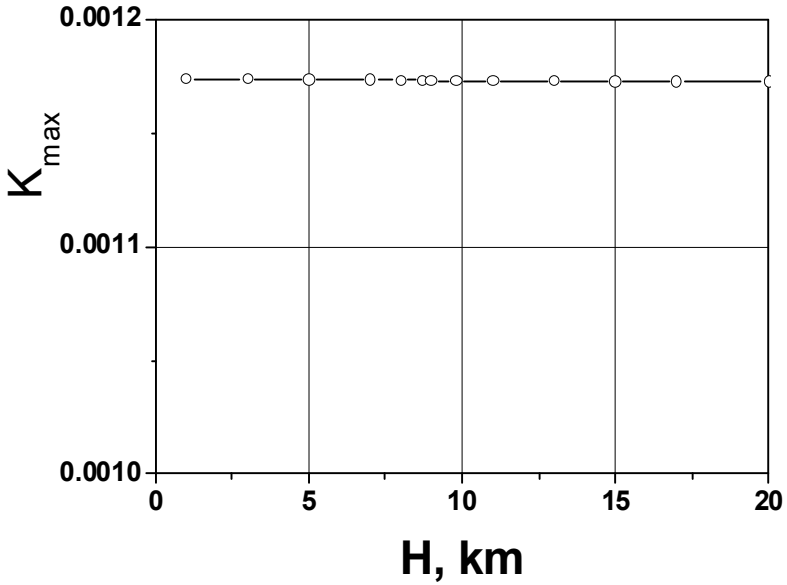
Conclusion: Absorbance is high enough to measure turbulence.

CO_2 channel

Tasks of CO_2 channel: CO_2 concentration and isotopes ratio measurements inside “Chernin” matrix optical system.

Parameters: L = 40 m, P = 100 mBar, Red - H_2O (15000 ppm), green - $C0_2$ (365 ppm), blue - CH_4 (1.8 ppm).

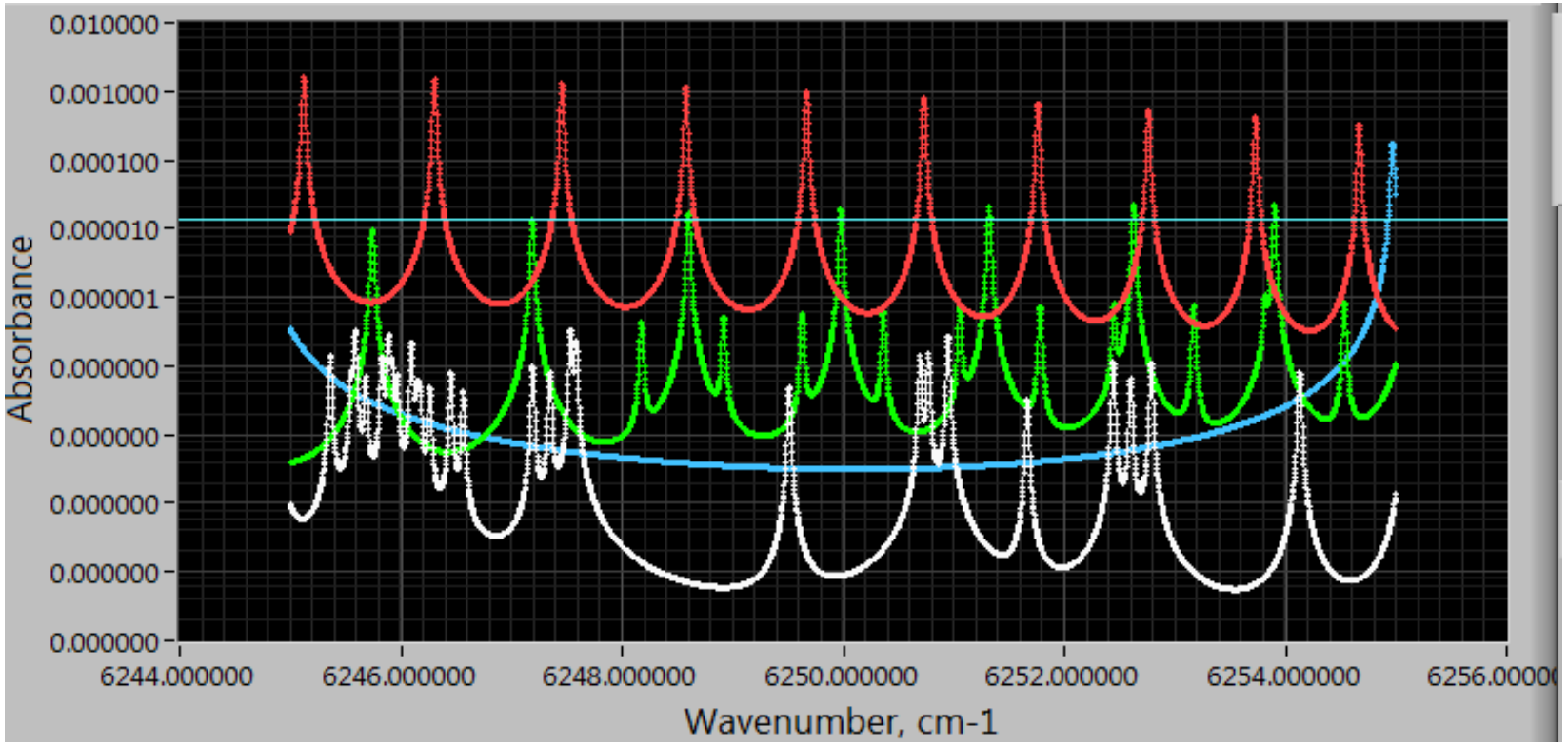




Isolated spectral line 6248.5779 cm^{-1} was selected as analytical one.
Left - analytical line max absorbance vs. altitude.

<u>Conclusion: Absorbance is high enough to measure CO_2 concentration for altitudes up to 25 km.</u>

Ratio $^{13}CO_2$:$^{12}CO_2$



Parameters: L = 40 m, P = 100 mBar, Red – $^{12}C^{16}O_2$ (365 ppm), green - $^{13}C^{16}0_2$ + $^{13}C^{16}O^{18}O$ (natural abundance), white - CH_4 (1.8 ppm).

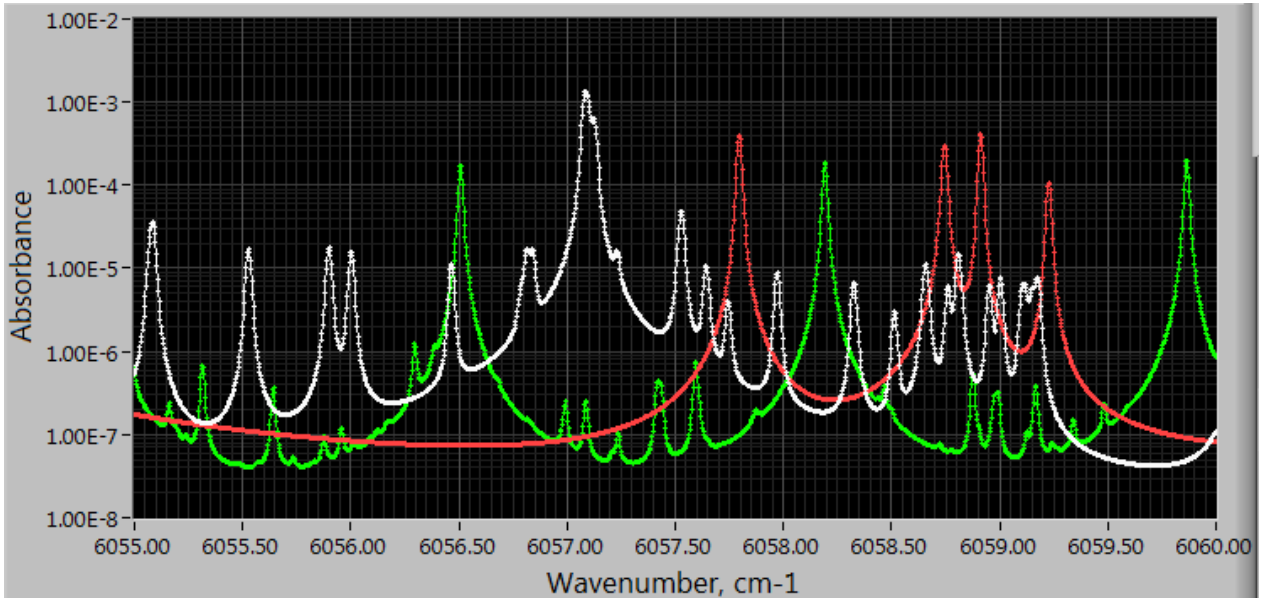
Spectral lines 6249.6694 and 6249.9753 cm^{-1} were selected as analytical ones to detect $^{12}C^{16}O_2$ and $^{13}C^{16}O_2$, respectively.

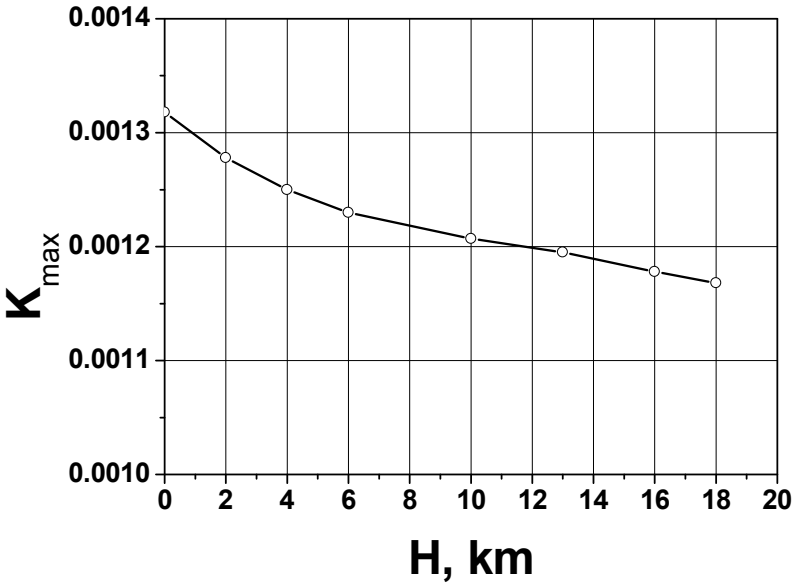
Conclusion: Absorbance is high enough to measure $^{13}C/^{12}C$ ratio for altitudes up to 25 km.

CH_4 channel

Task of CH_4 channel: measure CH_4 inside “Chernin” matrix optical system.

Parameters: L = 40 m, P = 100 mBar, blue - CH_4 (1.8 ppm), red - H_2O (15000 ppm), green - $C0_2$ (365 ppm).





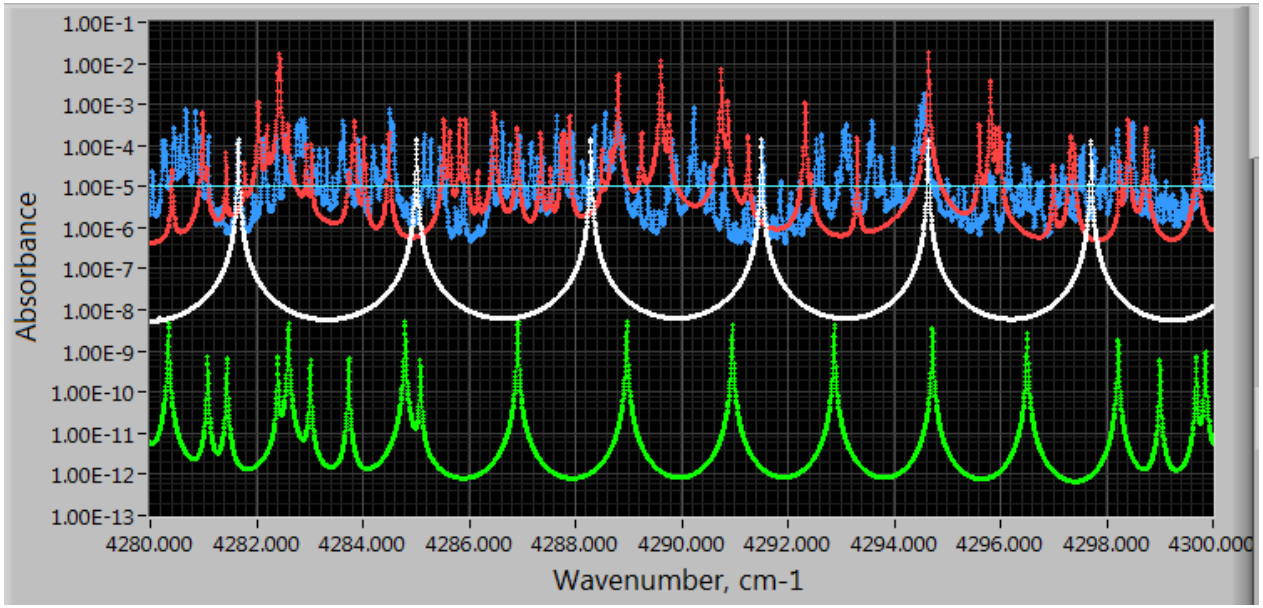
CH_4 multiplet 6057.08 cm^{-1} was selected as analytical line.
Left - analytical line max absorbance vs. altitude.

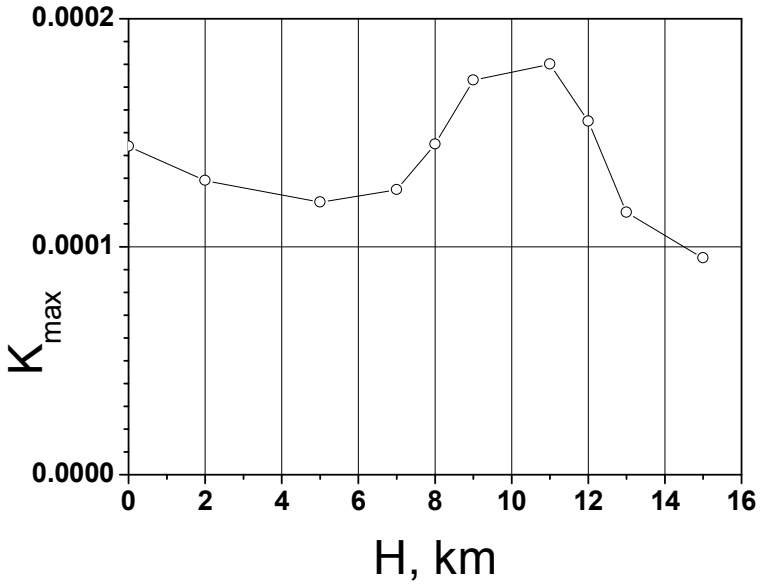
Conclusion: Absorbance is high enough to measure CH_4 concentration for altitudes up to 25 km.

CO channel

Task of CO channel: measure CO inside “Chernin” matrix optical system.

Parameters: L = 40 m, P = 100 mBar, white - CO (0.1 ppm), blue - CH_4 (1.8 ppm), red - H_2O (15000 ppm), green - $C0_2$ (365 ppm).





Spectral line 4291.4994 cm^{-1} was selected as analytical line.
Left - analytical line max absorbance vs. altitude.

Conclusion: Absorbance is high enough to measure CO concentration for altitudes up to 25 km.

Conclusion

Software “line-by-line” was developed to model atmosphere constituents spectra. Software developed is using molecular spectral data from HITRAN 2008 as well as atmosphere models available. Using software developed several atmosphere constituents (H_2O, CO_2, CO, CH_4) spectra altitude dependences were modeled.

Modeling performed shows:

1. Different water molecule isotopes can be detected up to 25 km altitude.
2. Water absorbance is high enough to measure atmosphere turbulence.
3. CO_2 concentration can be measured for altitudes up to 25 km.
4. $^{13}C/^{12}C$ ratio can be measured for altitudes up to 25 km.
5. CH_4 concentration can be measured for altitudes up to 25 km.
6. CO concentration can be measured for altitudes up to 25 km.