New Routine for Calculating the non-LTE CO_2 15 µm Cooling of Mesosphere and Lower Themosphere in GCMs

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Motivation

Any physical parameterization for GCM must be able to react as realistic as possible at steady changing local physical state of the atmosphere in the modeling process. This is particularly true for parametrizing the infra-red radiation and its effects (local cooling or heating), which are critically important for adequate modeling of energy balance. The instantaneous p-T distributions in modern GCMs of middle and upper atmosphere exhibit very strong variability, caused by the superposition of tidal and gravity waves of different amplitude and vertical scales. Therefore, the parameterization of the 15-micron CO_2 cooling, which is a main radiative cooling mechanism of these layers, must properly react to this variability.

However, the matrix parameterizations of the 15-micron cooling are unable to provide adequate reaction to strongly disturbed T distributions. This was well known already 30 years ago for those who worked on developing the first version of the Fomichev et al, 1998 routine.

Summary

We present a new routine KF23 for calculating the non-local thermodynamic equilibrium (non-LTE) 15 µm CO_2 cooling/heating of mesosphere and lower thermosphere in General Circulation Models (GCMs).

KF23 provides exact solution of the optimized models of the non-LTE in CO_2 for day and night conditions. It delivered cooling/heating with an error not exceeding 1 K/Day even for strong temperature disturbances. Compares to this the Fomichev et al, 1998 (F98) routine errors reach 25 K/day.

These errors may not be removed in the framework of the parameterization approach, as the revised version of the Fomichev-98 algorithm presented by Lopez-Puertas et al, (2023), shows (see also Kutepov, 2023).

KF23 uses exact algorithm based on the Accelerated Lambda Iteration (ALI) and Opacity Distribution Function (ODF) techniques for the non-LTE cooling/heating calculations, and is about 1000 faster than the standard matrix/line-by-line calculations.

Summary (continued)

KF23 has an interface for feed-backs from the model and is ready for implementation in any GCM.

KF23 may use any quenching rate coefficient of the CO2(v2)+O(3P) reaction, any O(3P) density and allows the user to vary the number of vibrational levels and bands to find a balance between the calculation speed and accuracy.

KF23 handles broad variation of CO_2 both below and above the current volume mixing ratio, up to 4000 ppm. This allows using this routine for modeling the Earth's ancient atmospheres and the climate changes caused by increasing CO_2.

Reference

Kutepov, A. and Feofilov, A.: New Routine NLTE15µmCool-E v1.0 for Calculating the non-LTE CO2 15 µm Cooling in GCMs of Earth's atmosphere, Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2023-115, in review, 2023.

The CO2 non-LTE day- and night-time models used the KF23 routine

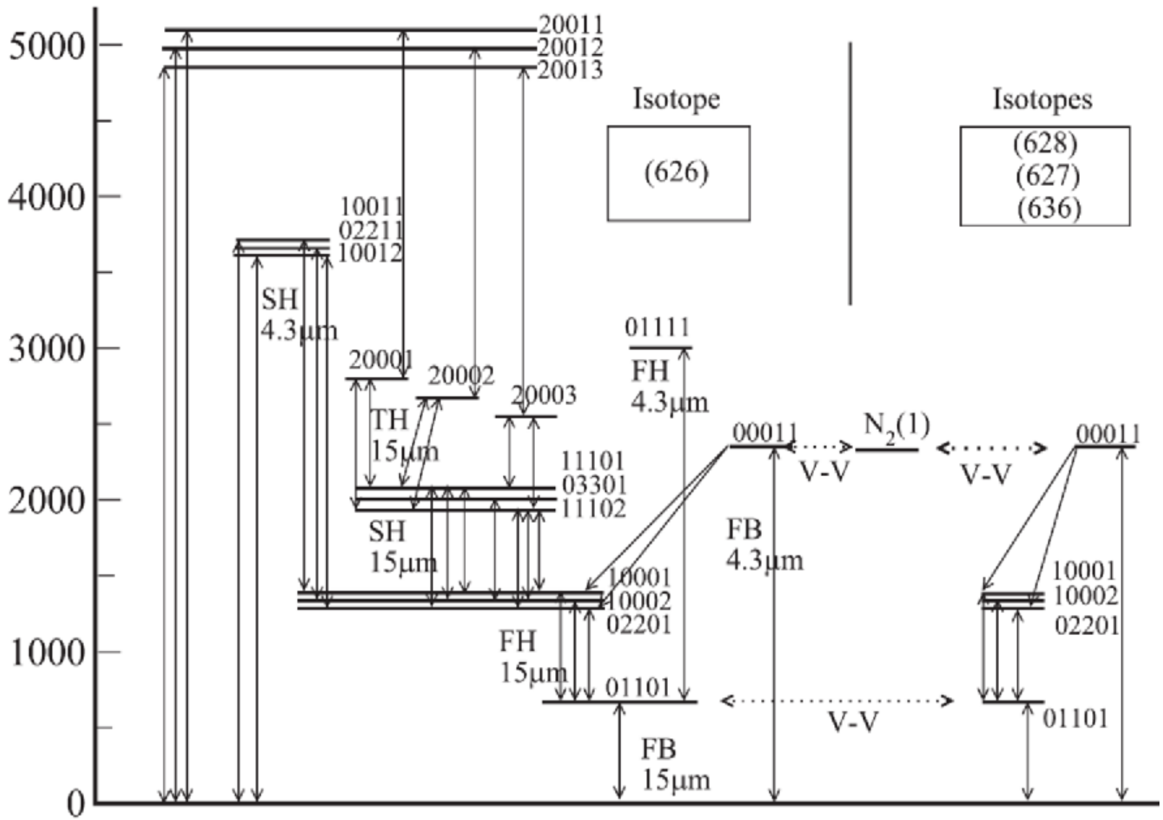


Table 1. CO_2 vibrational levels included in the night- and daytime model	
Isotope, HITRAN level notification, energy in cm-1	
626 00001 0.0	636 00001 0.0
626 01101 667.379960	636 01101 648.478030
626 10002 1285.40834	636 02201 1297.26326
626 02201 1335.13161	
626 10001 1388.18432	628 00001 0.0
626 11102 1932.47013	628 01101 662.37335
626 03301 2003.24615	
626 11101 2076.85588	627 00001 0.0
D 626 00011 2349.14291	627 01101 664.72941
D 626 01111 3004.01227	
D 626 10012 3612.84080	44 0 0.0
D 626 02211 3659.27229	D 44 1 2329.9116
D 626 10011 3714.78193	
D 626 20013 4853.62341	66 0 0.0
D 626 20012 4977.83500	D 66 1 1556.3519
D 626 20011 5099.66050	
	6 0 0.0
D marks levels added in daytime model	

Figure 1. CO2 vibrational levels diagram (Feofilov and Kutepov, 2012). Solid lines with arrows – main optical transitions, dashed lines with arrows - main V–V energy exchange processes, V–T transitions are not shown. Table 1 shows levels included new KF23 routine for night and day. Reverence model (not shown) includes 60 vibrational level of 5 CO2 isotopes and about 200 bands

Computational performance, comparison with other algorithms

Table 2. Numbers of operation and computing times. *Times are given in sec.*

NIGHT: NL=18; NB=18, NBr= 54, NRT=3078; NF=32; NA=2: ND=125; CO2x1

Night	N_{Aux}/T_{Aux}	N_{Rad} / T_{Rad}	N_{Inv} / T_{Inv}	N_I	T_{tot}	*K*
MM/LBL	2.8e5 / 5e-2	2.5e7 / 0.25	1.14e10/43	2	86	860
LI / ALI, LBL	5e4 / 8.5e-3	2.5e7 / 0.25	7.3e5/7.7.0e-3	60/5	16/1.3	160/ 13
ALI, ODF	5e4 / 8.5e-3	4.5e5 / 4.5e-3	7.3e5/7.7.0e-3	5	0.1	1

DAY: NL=28; NB=46, NBr= 119, NRT=6039; NF=32; NA=2: ND=125; CO2x1

Day	N_{Aux}/T_{Aux}	N_{Rad} / T_{Rad}	N_{Inv} / T_{Inv}	N_I	T_{tot}	*K*
MM/LBL	4.4e5/2e-1	4.8e7/0.48	4.3e10/160	2	321	1284
LI / ALI, LBL	1.1e5/1.9e-2	4.8e7/0.48	2.7e6/2.2e-2	60/5	31/2.6	124/10
ALI, ODF	1.1e5/1.9e-2	9.5e5/9.5e-3	2.7e6/2.2e-2	5	0,25	1

New Routine KF23 (ALI/ODF in the table) calculate the cooling 860 times faster for night and 1286 times faster for day than the standard matrix method + line-by-line radiative transfer (MM/LBL in the table). For details see the paper at https://doi.org/10.5194/gmd-2023-115

Accuracy of cooling/heating rate calculations (1)

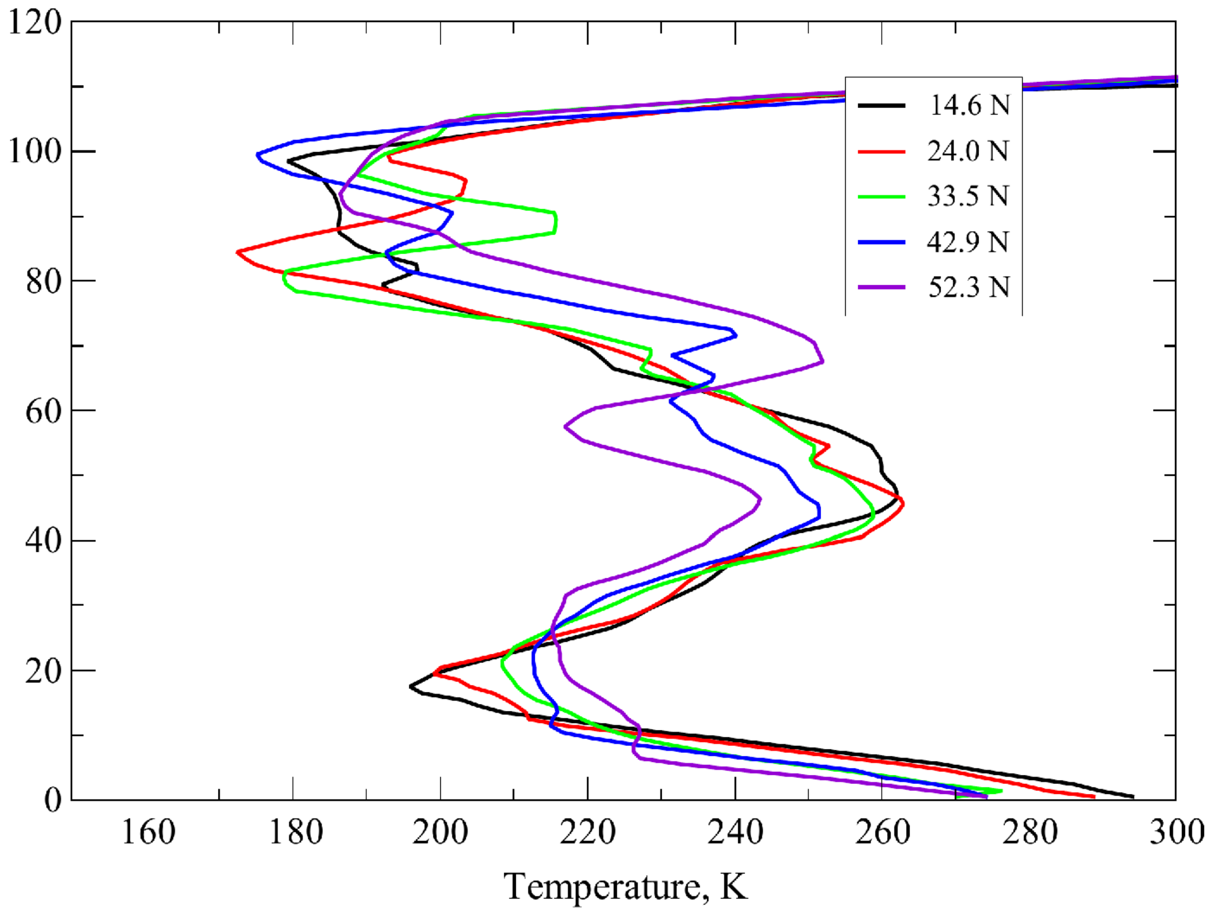


Figure 2. WACCM6 CESM generated temperature profiles used for testing the accuracy of the CO2 15 µm cooling calculations

Accuracy of cooling/heating rate calculations (2)

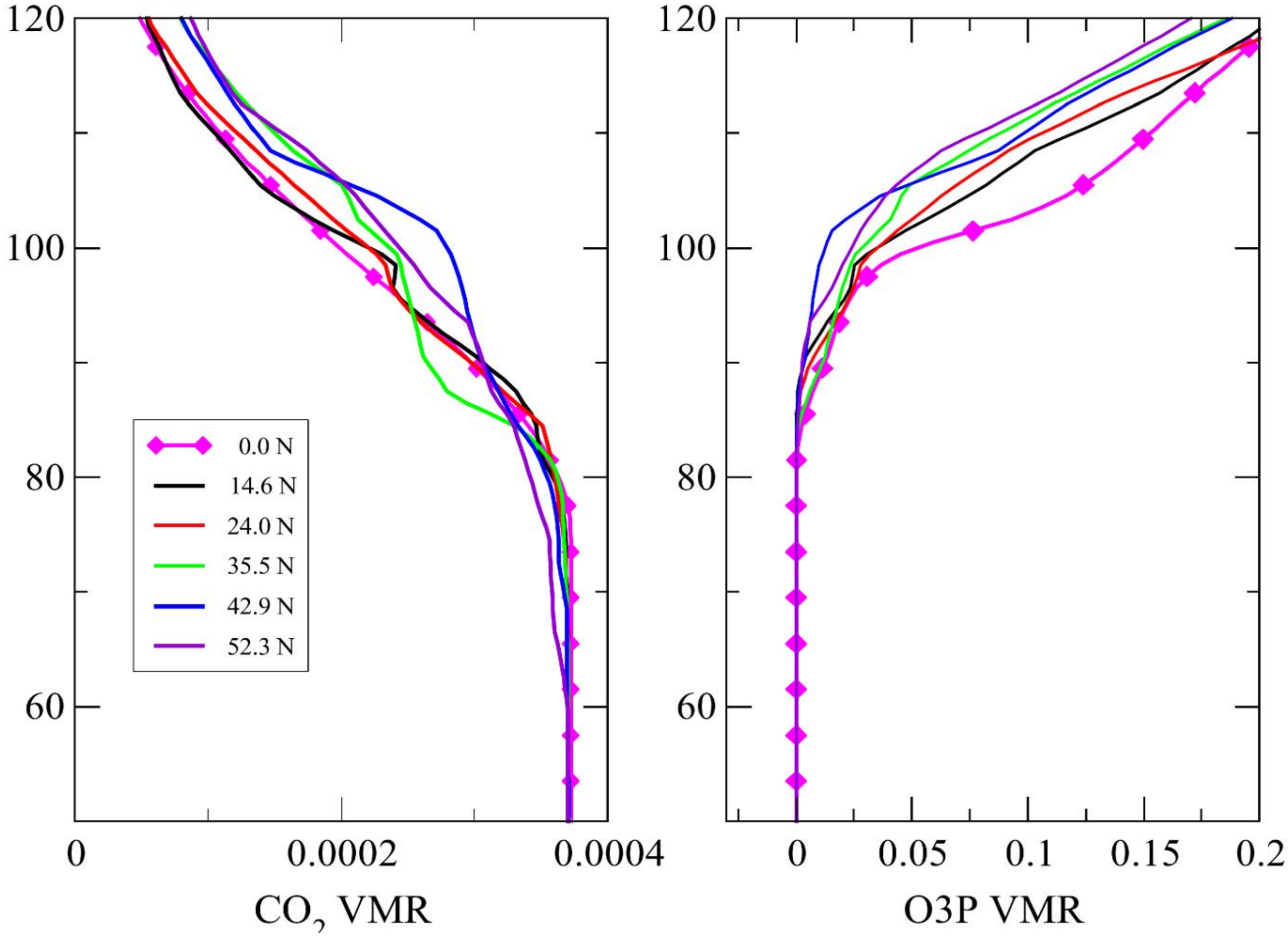
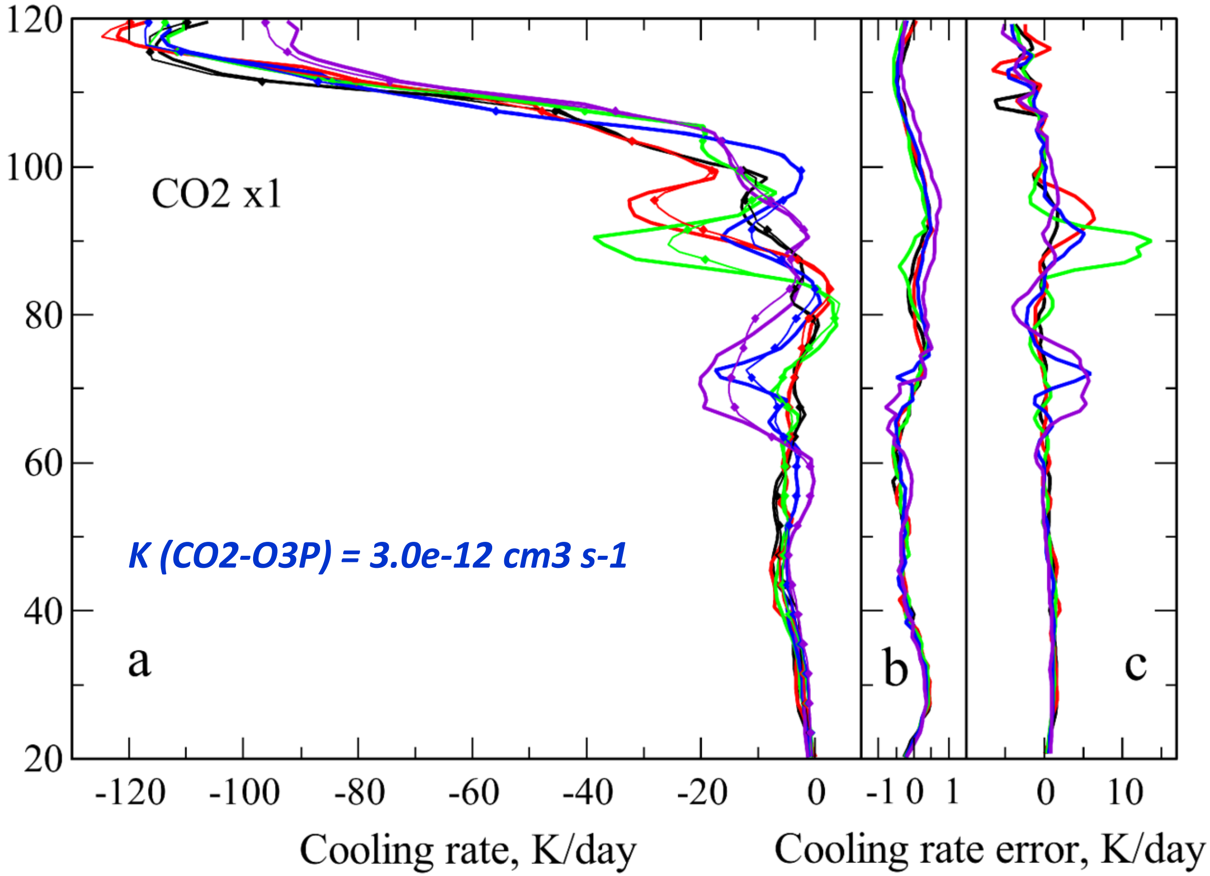


Figure 3. WACCM6 CESM CO2 and O3P vmr profiles used for testing the accuracy of the CO2 15 µm cooling calculations. Magenta with diamonds shows data from Yudin et al, 2022 for diurnal tides at equator.

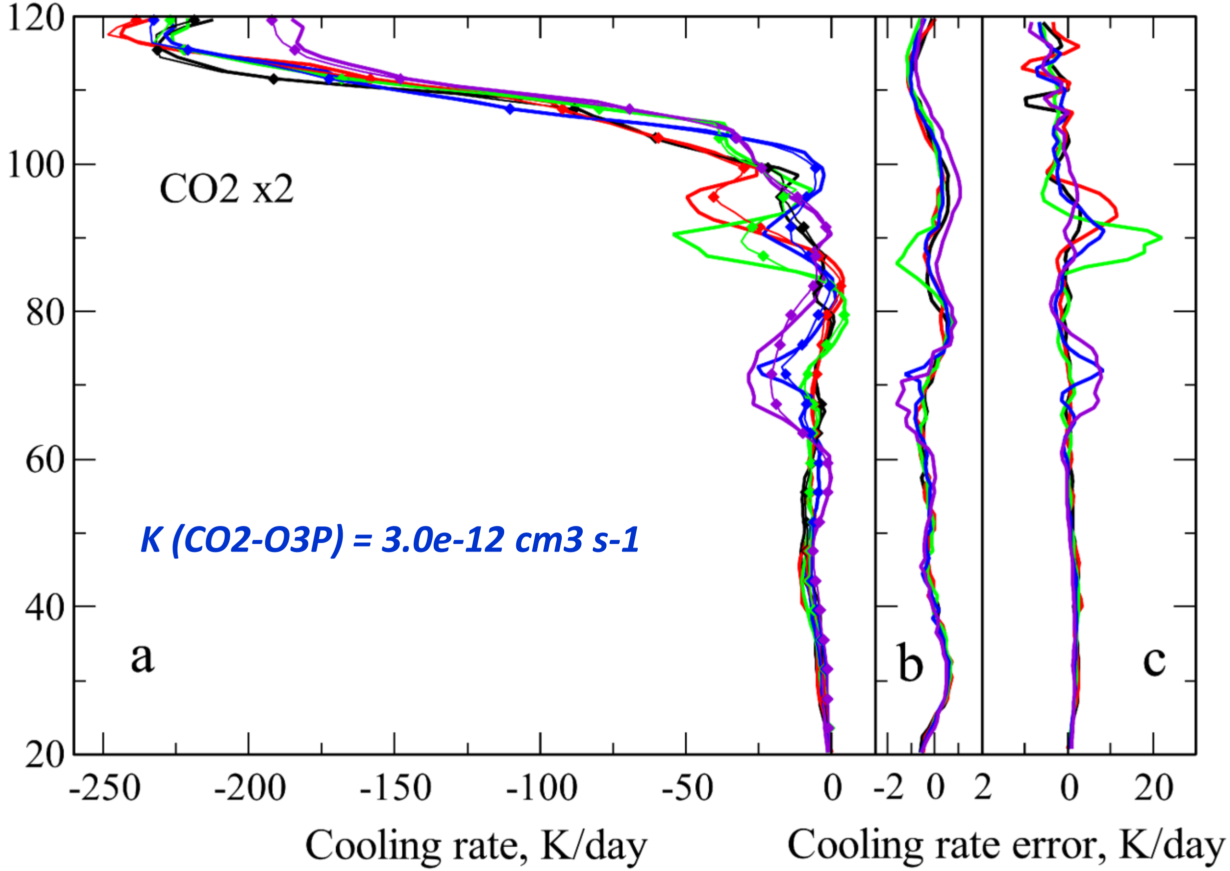
Accuracy of cooling/heating rate calculations (4)



Cooling errors of the Fomichev et al. 1998 routine (F98) around mesopause exceed 10 K/Day. Errors of new KF23 routine are < 1 K/Day for all altitudes.

Figure 4. Cooling rates in the CO_2 15 µm band and cooling rates errors for the CO_2 VMR of 400 ppm for inputs shown in Figs. 2 and 3. (a): Thick solid lines - reference data (REF); thin solid lines with diamonds – Fomichev et al 1998 (F98); (b) new routine of Kutepov and Feofilov, 2023 (KF23) minus REF; (c) F98 minus REF.

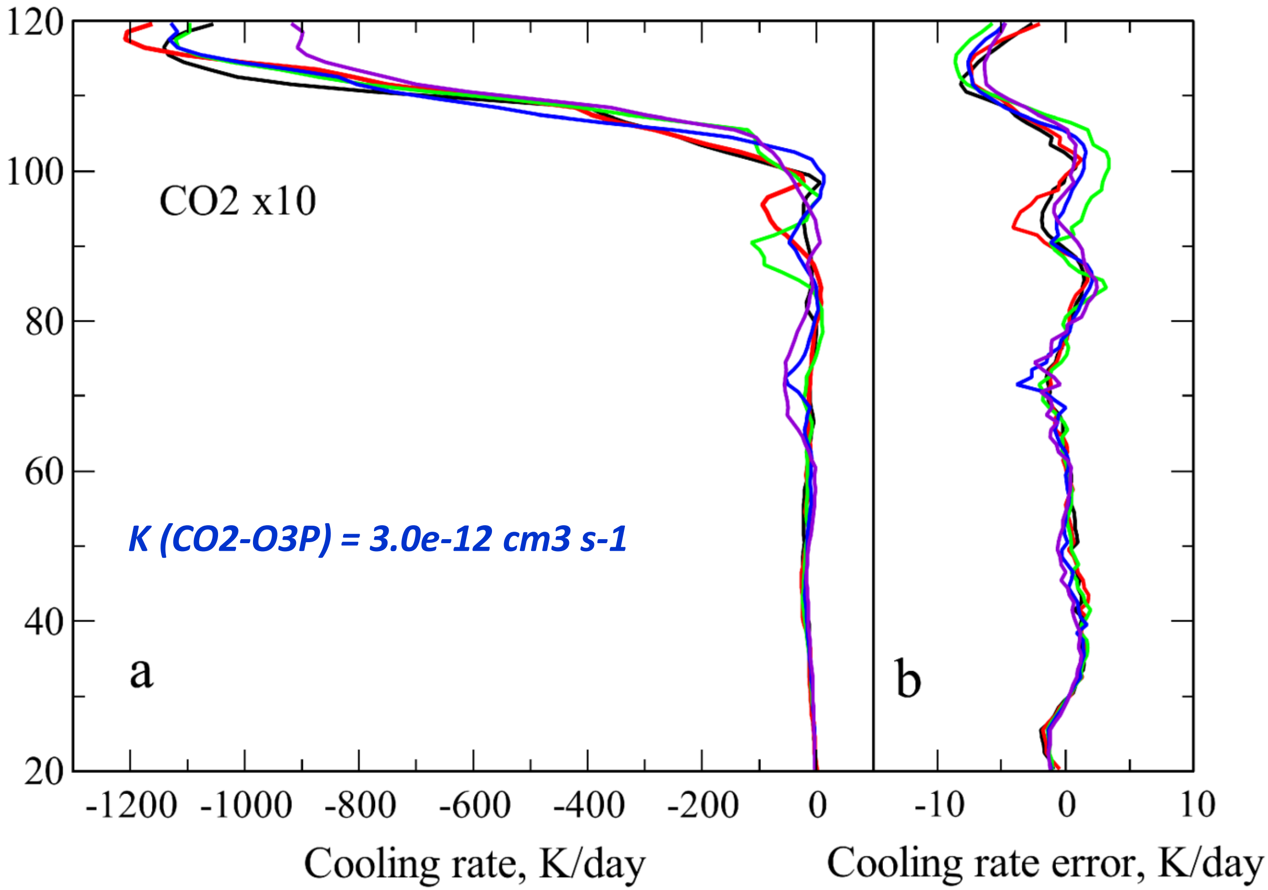
Accuracy of cooling/heating rate calculations (5)



Cooling errors of the Fomichev et al. 1998 routine (F98) around mesopause reach 20 K/Day. Errors of new KF2023 routine are < 2 K/Day for all altitudes .

Figure 5. Cooling rates in the CO_2 15 μm band and cooling rates errors for the CO_2 VMR of 800 ppm for inputs shown in Figs. 2 and 3. (a): Thick solid lines - reference data (REF); thin solid lines with diamonds – Fomichev et al 1998 (F98); (b) new routine of Kutepov and Feofilov, 2023 (KF23) minus REF; (c) F98 minus REF.

Accuracy of cooling/heating rate calculations (6)



Errors of new KF2023 routine are < 10 K/Day for all altitudes .

Figure 7. Cooling rates in the CO2 15 µm band and cooling rates errors for the CO2 VMR of 4000 ppm for inputs shown in Figs. 2 and 3. (a): Thick solid lines - reference data (REF); (b) new routine of Kutepov and Feofilov, 2023 (KF23) minus REF;

Accuracy of cooling/heating rate calculations (6)

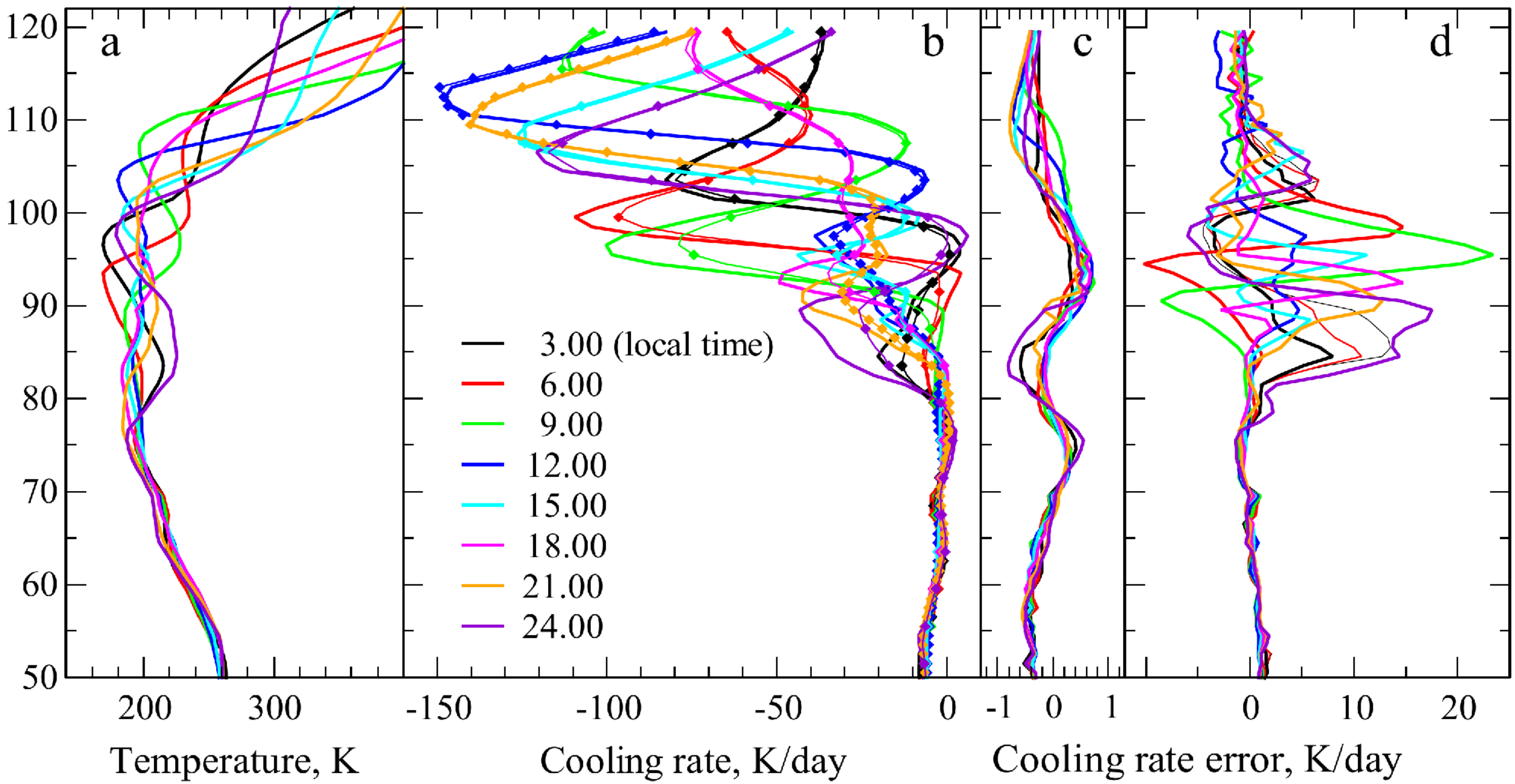


Figure 9. CO2 15 µm cooling rates for diurnal tides at equator. (a) Temperature profiles; (b) Cooling rates: thick solid lines - reference model (REF), thin solid lines with diamonds - F98 routine; (c) New KF23 routine minis REF; (d) F98 routine minis REF. ***The errors of Fomichev et al, 1998 routine (F98) reach 25 K/Day near the mesopause.***

Conclusion

We present the new KF23 routine for calculating the non-LTE CO2 15 µm radiative cooling/heating in the GCMs of middle and upper Atmosphere

- ***KF23 delivers high accuracy cooling rates for any temperature distributions including those disturbed by strong micro- and meso-scale strictures:***

Maximal errors of the 15 µm radiative cooling/heating for Fomichev et al, 1998 routine (F98) and Kutepov and Feofilov 2023 routine (KF23) for smooth/wave disturbed T profiles (in K/Day)

CO2 vmr	F98	KF23
400 ppm	1-2 / 25	0.2 / 1
800 ppm	2-4 / 47	0.3 / 2
1600 ppm	---	0.7 / 3.5
4000 ppm	---	1.5 / 10

- ***KF23 routine provides accurate cooling calculations in a very broad ranges of CO2(v2)- O(3P) quenching rate and O(3P) variation.***

Conclusion (continued)

- ***KF23 routine provides accurate cooling calculations in a very broad ranges of CO2(v2) - O(3P) quenching rate and O(3P) variation.***

- ***KF23 works for very broad variation of CO2 both below and above the current density, up to 4000 ppm. This allows using this routine for modeling the Earth's ancient atmospheres and the climate changes caused by increasing CO2 .***

- ***Recently Lopez-Puertas et al., 2023 tried to update the parameterization of Fomichev et al, 1998. Unfortunately, the attempt to improve the parameterization accuracy failed (see Kutepov, 2023 for detailed analysis): for wavy temperature profiles the revised routine works no better that the standard Fomichev-1998 routine.***

References

- *Fomichev, V. I., Blanchet, J.-P., and Turner, D. S.: Matrix parameterization of the 15 µm CO2 band cooling in the middle and upper atmosphere for variable CO2 concentration, Journal of Geophysical Research: Atmospheres, 103, 11 505–11 528, https://doi.org/10.1029/98jd00799, 1998.*
- *Kutepov, A. and Feofilov, A.: New Routine NLTE15µmCool-E v1.0 for Calculating the non-LTE CO2 15 µm Cooling in GCMs of Earth's atmosphere, Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2023-115, in review, 2023*
- *Kutepov, A. A., Comment to "An improved and extended parameterization …" by López-Puertas, M., et al, 2023 ', https://egusphere.copernicus.org/preprints/2023/egusphere-2023-2424/egusphere-2023-2424-CC1-supplement.pdf. 2023.*
- *López-Puertas, M., et al. An improved and extended parameterization of the CO2 15 µm cooling in the middle/upper atmosphere, https://doi.org/10.5194/egusphere-2023-2424 Preprint. Discussion started: 6 November 2023.*