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Absorption of infrared radiation by carbon monoxide at elevated temperatures and pressures: Part A. Advancing the line-by-line procedure based on HITEMP-2010



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ABSTRACT

A line-by-line procedure has been developed for calculating the effective band width (band absorptance) of both the fundamental and the first overtone bands of carbon monoxide. The procedure is based on HITEMP-2010 data base and each absorption line has been truncated to remedy the sub-Lorentzian behavior in the line wings. The truncation criterion has been given in the paper. The line-by-line procedure has been used to reproduce all available (published) measured CO-absorption spectra. The calculated effective band width for the fundamental band is within 10% of the measured values while that for the 1st overtone is within 5% margin for CO pressures as large as 70–80 bar and temperatures not larger than 600 K. For temperatures larger than 600 K and approaching 2700 K, the line-by-line procedure provides the effective band widths that can be as much as 30% lower than those calculated using the measured spectra. The higher the temperature the larger is the difference between the measured and calculated spectra.

Scrutiny of the high-temperature CO absorption spectra has indicated inconsistency of the measured data and their inaccuracy in particular at larger wavenumbers. Thus, it is plausible that the accuracy of the line-by-line procedure is better than 30%. For a precise determination of the accuracy, the CO absorption measurements should be repeated using modern spectroscopy.

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1. Introduction and objectives

Absorption of infrared radiation by carbon monoxide (CO) is relevant in astrophysics (planetary atmospheres) as well as in utilization of various fuels. The CO fundamental band, located at 2143 cm^{-1} lies in the atmospheric window between the strong fundamental 2350 cm^{-1} CO₂ band and the 1600 cm^{-1} H₂O band. Not surprisingly CO absorption has been a subject of intensive research in conjunction with both remote sensing of the terrestrial atmosphere and atmospheric carbon cycle [1]. Carbon monoxide is a minor contributor to the Earth's greenhouse gas effect and is often neglected in such considerations [2]. Also in heat transfer calculations concerning combustion, the contribution of CO is often omitted since, in flames or in combustion chambers, CO is present in percentage level in not too large a volume of the flame. In post-combustion gases CO typically occurs in ppm levels. The situation is very different as far as gasification technology is concerned

where the objective is to produce a syn-gas containing typically 30–40% CO. Bioliq® gasifier [3,4], operating at 40 bar pressure is an example of such a reactor producing high pressure syn-gas from a biomass feedstock. Numerical simulations of such a gasifier require knowledge of CO absorption at elevated temperatures and pressures. Either absorption coefficients or narrow-band models or Weighted-Sum-of-Gray-Gas-Models or other correlations are needed to calculate the in-gasifier heat transfer.

In astrophysics, absorption of infrared radiation by CO molecule has thoroughly been investigated at temperatures not exceeding 310 K. The decades lasting research, not only on CO but many other molecules, has culminated in HITRAN [5] database where parameters of 4477 CO absorption lines are listed at 296 K temperature. For applications requiring temperatures in excess of 500 K, HITEMP database is currently under continues development and improvement [6]. In this work we use HITEMP-2010 to generate the CO absorption coefficients. The final goal (see Part B [7]) is to produce a total emissivity graph for CO molecule at 1 bar (atmospheric) pressure and provide a methodology for scaling the graph to pressures as high as 40 bar. Since HITEMP is a database under development it is imperative that the base is validated and to this

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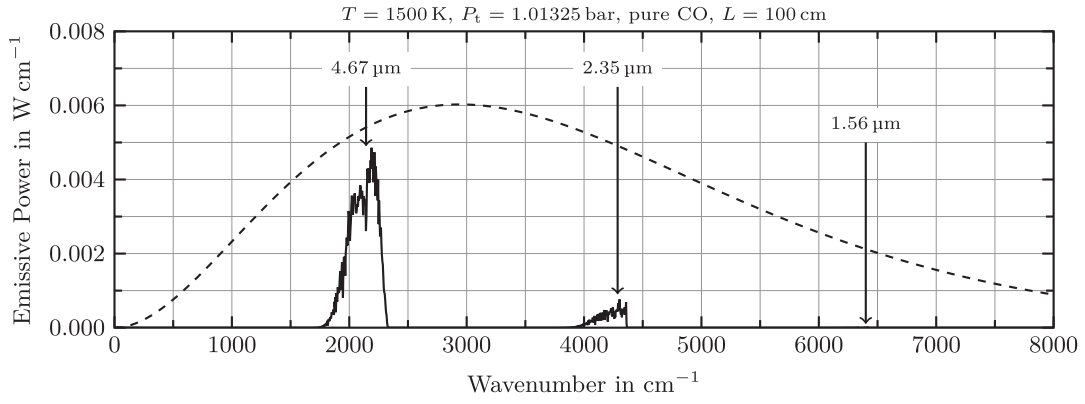


Fig. 1. Example of line-by-line calculations of spectral emissive power of carbon monoxide. The main absorption bands are marked within the spectrum, see also Table 1. The second overtone band is so weak that it is almost zero at $L = 100$ cm. Dotted line - Planck's function at 1500 K.

Table 1
Major infrared vibration-rotation bands of Carbon Monoxide [8].

Fundamental Vibration Mode		Wavenumber (cm^{-1})	Statistical Degeneracy
Stretching		$\eta_1 = 2143 \text{ cm}^{-1}$	$g_1 = 1$
λ_0 in μm	η_0 in cm^{-1}	δ	Type
4.67	2143	1	Fundamental η_1
2.35	4286	2	First Overtone
(1.56)	(6429)	(3)	(Second Overtone)

end we use a large set of data (see below). It will be demonstrated later that adjustments (cutting off the absorption lines to eliminate excessive absorption in the wings) are mandatory to reproduce the measured spectra. Thus, the objectives of this work (Part A) are twofold: (i) to develop a line-by-line procedure based on HITEMP-2010 database for CO molecule and (ii) to establish accuracy of the procedure in calculating effective band width (band absorbance) for both the fundamental and the 1st overtone bands. In Part B [7] we produce CO total emissivity graphs.

The infrared absorption spectrum of carbon monoxide mainly consists of the fundamental $4.67 \mu\text{m}$ -band corresponding to the fundamental vibration mode (stretching) and the combined rotation-vibration (first overtone) band located at $2.35 \mu\text{m}$. The second overtone, located at $1.56 \mu\text{m}$, hardly contributes to the total gas emissivity since it is very weak. Fig. 1 shows an example calculation using HITEMP-2010 [6] database. The individual bands are marked within the spectrum and are also listed in Table 1.

2. Research methodology

The integrated (total) emissivity of pure CO is calculated as follows:

$$\varepsilon^{\text{tot}}(T, p_{\text{CO}} \cdot L, P_t) = \frac{\dot{\varepsilon}_{\eta, \text{b}}(T, \eta_f)}{\sigma \cdot T^4} \cdot W_f + \frac{\dot{\varepsilon}_{\eta, \text{b}}(T, \eta_o)}{\sigma \cdot T^4} \cdot W_o \quad (1)$$

where T is the temperature in K, P_t is the total pressure in atm, and $p_{\text{CO}} \cdot L$ is the pressure path length or optical density in $\text{atm} \cdot \text{cm}$; W_f and W_o stand for the absorbance (in cm^{-1}) of the fundamental and the first overtone, respectively. It is assumed here that the variations of the Planck's function within the bands are negligible. The spectral blackbody emissive power ($\dot{\varepsilon}_{\eta, \text{b}}$) is calculated using the Planck's law

$$\dot{\varepsilon}_{\eta, \text{b}} = \frac{C_1 \cdot \eta^3}{\exp\left(\frac{C_2}{T \cdot \eta}\right) - 1} \quad (2)$$

so that $\dot{\varepsilon}_{\eta, \text{b}}$ is in $\text{W}/(\text{cm}^2 \cdot \text{cm}^{-1})$ when the wavenumber η is entered in cm^{-1} and the Planck's first and second constants are

$C_1 = 3.74178 \cdot 10^{-12} \text{ W cm}^{-2}$ and $C_2 = 1.43877 \text{ cm K}$. For the fundamental band, the band center is at $\eta_f = 2143 \text{ cm}^{-1}$ whilst the first overtone is located at $\eta_o = 4286 \text{ cm}^{-1}$.¹ It should be noted that Eq. (1) is valid because the individual absorption bands are well separated so that they do not overlap.

The band absorbance, or equivalent width W , appearing in Eq. (1) is calculated using

$$W = \int_{\eta_1}^{\eta_2} [1 - \exp(-a_\eta \cdot L)] \cdot d\eta = \int_{\eta_1}^{\eta_2} [1 - \tau_\eta] \cdot d\eta \quad (3)$$

The integration range from η_1 to η_2 must be wide enough to cover the whole band. Eq. (3) can be used for both the fundamental and the first overtone bands. For the integration, values of the absorption coefficient a_η are needed and they are calculated using HITEMP-2010 [6] spectral data base; an assembly of parameters describing each individual absorption line. The parameters are listed at 1 atm pressure and 296 K temperature. The methodology of scaling the lines into pressures different from 1 atm and temperatures different from 296 K is known, e. g. see Refs. [9,10] and the references therein, and to this end the software, described in our previous publications [9–11], has been used. The Voigt line profile at 0.001 cm^{-1} spectral resolution is used for pressures below atmospheric while Lorentz lineshape is applied elsewhere with 0.01 cm^{-1} resolution. Each spectral line is evaluated until the absorption coefficient is smaller than 10^{-9} cm^{-1} . While performing the line-by-line calculations care must be exercised in the wings of each absorption line. It has been known for long [12,13] that the Voigt / Lorentz function may overestimate the absorption in the far wings and this effect is often named as the existence of sub-Lorentzian wings. There are several ways to remedy the deficiency of the Voigt (Lorentz) line-shape function. The simplest way is to cut off the line at an arbitrarily chosen wavenumber away from the line center. In the nineties of the last century, in calculations of carbon dioxide absorption, the line wings were truncated

¹ The band centres are taken here as quoted in the classical literature [8] on CO spectra.

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