On the accuracy of HITEMP-2010 calculated emissivities of Water Vapor and Carbon Dioxide

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\[
K_{\alpha,\eta} (\eta; T, P_t, x_j, L) = S_H(T) \cdot N(p_j, T) \cdot g(\eta - \eta_i)
\]

- 7 Parameter for each line are needed from Spectral database
- Equation of state: Ideal gas law
- Lineshape: Lorentz
- \( a_{\eta} = \sum_{\text{all lines}} K_{\alpha,\eta} \)
Line-by-Line Method

\[ T = 1800 \text{ K}, \ P_t = 1 \text{ atm}, \text{ pure CO}_2, \ L = 50 \text{ cm} \]

\[ \tau_\eta = \exp (-a_\eta \cdot L) \]

\[ \varepsilon_\eta = 1 - \tau_\eta \]
Line-by-Line Method

$T = 1800\, \text{K}, \quad P_t = 1\, \text{atm}, \quad \text{pure H}_2\text{O}, \quad L = 50\, \text{cm}$

$\varepsilon^{\text{tot}} = \frac{1}{\sigma \cdot T^4} \cdot \int_{0}^{\infty} \varepsilon_\eta \cdot \frac{c_1 \cdot \eta^3}{\exp \left( \frac{c_2 \cdot \eta}{T} \right) - 1} \cdot d\eta$
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Important Measurements (without any claim to completeness)

- Modest & Bharadwaj (2002-2007) [5, 6, 10]
  - up to 1550 K, CDSD-1000 and HITEMP-1995, 4 cm\(^{-1}\)
  - also compared with HITEMP-2010, see Alberti et. al. [1]

- Becher et. al. (2012) [4]
  - up to 1770 K, HITEMP-2010, Measurements performed at DTU, 32 cm\(^{-1}\)

- Alberti et. al. (2015) [3]
  - 22 cases, 500 - 1770 K, also mixtures, DTU, 1 cm\(^{-1}\)
  - whole spectral range from 450 to 7600 cm\(^{-1}\)
High Temperature - Alberti et. al. (2015)

$\text{CO}_2 \text{ at } 1770 \text{ K}, \ x_{\text{CO}_2} = 0.43, \ x_{\text{N}_2} = 0.57, \ P_t = 1 \text{ atm}, \ L = 54 \text{ cm}$

Difference $= \mathcal{T}_\eta,\text{Measured} - \mathcal{T}_\eta,\text{HITEMP–2010}$

see Alberti et. al. [3]
High Temperature - Alberti et. al. (2015)

$H_2O$ at 1770 K, $x_{H_2O} = 0.43$, $x_{N_2} = 0.57$, $P_t = 1$ atm, $L = 54$ cm

$\tau_{\eta}$, Measured $-$ $\tau_{\eta}$, HITEMP–2010

see Alberti et. al. [3]
High Temperature - Alberti et. al. (2015)

H$_2$O and CO$_2$ at 1770 K, $x_{H_2O} = x_{CO_2} = 0.43$, $P_t = 1$ atm, $L = 54$ cm

Difference = $\tau_\eta,\text{Measured} - \tau_\eta,\text{HITEMP-2010}$

see Alberti et. al. [3]
High Temperature - Alberti et. al. (2015)

CO₂ Emissivity Chart, $x_{CO₂} = x_{N₂} = 0.5$

$\begin{align*}
\text{Total Emissivity} & \quad \text{Temperature in K} \\
0.20 & \quad 400 \quad 600 \quad 800 \quad 1000 \quad 1200 \quad 1400 \quad 1600 \quad 1800 \quad 2000 \\
0.15 & \quad 55 \text{ bar cm} \\
0.10 & \quad 38 \text{ bar cm} \\
0.05 & \quad 24 \text{ bar cm} \\
0.00 & \quad 9 \text{ bar cm}
\end{align*}$

- $pL = p_{CO₂} \cdot L$
- Calculated using HITEMP-2010
- × Calculated using Measurements of Alberti et. al. (2015)
High Temperature - Alberti et. al. (2015)

\[ H_2O \text{ Emissivity Chart, } x_{H_2O} = x_{N_2} = 0.5 \]

Temperature in K

Total Emissivity

\[ pL = p_{H_2O} \cdot L \]
High Temperature - Alberti et. al. (2015)

\[ (p_{CO_2} + p_{H_2O}) \cdot L = 47 \text{ bar cm} \]

\[ \frac{p_{H_2O}}{p_{CO_2}} = 4.0 \]

\[ \frac{p_{H_2O}}{p_{CO_2}} = 4.0 \]

\[ 1.0 \]

\[ 0.25 \]

\[ pL = (p_{CO_2} + p_{H_2O}) \cdot L \]

Calculated using HITEMP-2010

Calculated using Measurements of Alberti et. al. (2015)
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Important Results for CO$_2$ (without any claim to completeness)

- **Measurements**
  - Fukabori et. al. (1986) [7]
  - Hartmann and Perrin (1989) [8, 11]
  - Scutaru et. al. (1993) [12]

- **Models/Adjustments**
  - Full Line-Mixing software of Lamouroux [9]
  - $\chi$-factors of Tran (2011) [13]
  - Cut-off criterion of Alberti et. al. (2015) [2]
    - Number Lorentz-half-widths

\[
n(T, P_t) = 4.0 \cdot \left(\frac{T}{P_t}\right)^{0.822}
\]
High Pressure - Alberti et. al. (2015)

$T = 303\, \text{K}, P_t = 11.1\, \text{bar}, \text{pure CO}_2, L = 5.02\, \text{cm}$

Transmissivity $\tau$

Wavenumber in cm$^{-1}$

See also Ref. [2]
High Pressure - Alberti et. al. (2015)

$T = 623 \text{ K}, P_t = 52 \text{ bar}, \text{pure CO}_2, L = 4.4 \text{ cm}$

Transmissivity $\tau_n$

see also Ref. [2]
High Pressure - Alberti et. al. (2015)

Temperature $T = 300$ K

Total Emissivity vs. Total pressure in bar

- No Limit
- Limited
- $\chi$-Tran (2011)
- FLM

see also Ref. [2]
High Pressure - Alberti et. al. (2015)

Temperature $T = 1500$ K

Total Emissivity

Total pressure in bar

No Limit Limited $\chi$-Tran (2011)

see also Ref. [2]
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Summary and Conclusion

- High temperature and atmospheric pressures
  - $\text{CO}_2$: maximum 2% difference (up to 1770 K)
  - $\text{H}_2\text{O}$: maximum 9% difference (up to 1770 K)
  - $\text{CO}_2 + \text{H}_2\text{O}$: maximum 7% difference (up to 1770 K)

- High pressure / density
  - Measurements for small spectral regions
  - New, full spectrum measurements are needed
  - Lineshape adjustment seems to be essential

- CO measurements for gasification applications
Acknowledgments

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Bibliography I


Appendix

The gas cell design can be traced back to Hottel & Mangelsdorf (1935). [3]
### Appendix

\[ \tau_\eta = \frac{(I_{\text{hot\ gas}} - I_{\text{cold\ gas}})}{(I_{\text{hot\ N}_2} - I_{\text{cold\ N}_2})} \]

See also Ref. [3]
Appendix

Transmissivity $\tau = 1770.15$ K, $x_{H_2O} = 0.9811$, $P_t = 1.0262$ atm, $L = 54.00$ cm, Voigt Lineshape

See also Ref. [3]