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

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

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

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

\[ \tau_\eta = \exp (-a_\eta \cdot L) \quad \epsilon_\eta = 1 - \tau_\eta \]
Line-by-Line Method

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

Transmissivity $\tau$ is plotted against wavenumber in cm$^{-1}$.

Wavenumbers and corresponding transmissivity values:
- $>10 \mu\text{m}$
- $6.3 \mu\text{m}$
- $2.7 \mu\text{m}$
- $1.87 \mu\text{m}$
- $1.38 \mu\text{m}$

The transmissivity equation is given by:

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

- Modest & Bharadwaj (2002-2007) [5, 6, 11]
  - 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)

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

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

see Alberti et. al. [3]
Transmissivity $\tau$ of $H_2O$ at 1770 K, $x_{H_2O} = 0.43$, $x_{N_2} = 0.57$, $P_t = 1$ atm, $L = 54$ cm

\[
\text{Difference} = \tau_{\eta,\text{Measured}} - \tau_{\eta,\text{HITEMP–2010}}
\]

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

$H_2O$ 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]
CO$_2$ Emissivity Chart, $x_{CO_2} = x_{N_2} = 0.5$

- Calculated using HITEMP-2010
- × Calculated using Measurements of Alberti et al. (2015)

$$pL = p_{CO_2} \cdot L$$
High Temperature - Alberti et. al. (2015)

$H_2O$ Emissivity Chart, $x_{H_2O} = x_{N_2} = 0.5$

$pL = p_{H_2O} \cdot L$

Calculated using HITEMP-2010

Calculated using Measurements of Alberti et. al. (2015)
High Temperature - Alberti et. al. (2015)

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

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

\[ \frac{p_{H_2O}}{p_{CO_2}} = 1.0 \]

\[ \frac{p_{H_2O}}{p_{CO_2}} = 0.25 \]

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

- Calculated using HITTEMP-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, 12]
  - Scutaru et. al. (1993) [13]

- **Models / Adjustments**
  - Full Line-Mixing software of Lamouroux [10]
  - $\chi$-factors of Tran (2011) [14]
  - 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

Important Results for CO$_2$ (without any claim to completeness)

- **Measurements**
  - Fukabori et. al. (1986) [7]
  - Hartmann and Perrin (1989) [8, 12]
  - Scutaru et. al. (1993) [13]

- **Models / Adjustments**

  Line-Mixing (finite duration of collision)

![Graph showing absorption vs. wavenumber](Taken from Hartmann [9])
High Pressure

Important Results for CO₂ (without any claim to completeness)

- **Measurements**
  - Fukabori et. al. (1986) [7]
  - Hartmann and Perrin (1989) [8, 12]
  - Scutaru et. al. (1993) [13]

- **Models / Adjustments**

  Adjustments for Lorentz / Voigt Lineshape

\[
\eta_i \cdot \chi (T, P_t) \cdot \Delta \cdot \log K_{a,\eta}
\]
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 $\tau$

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

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

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

Temperature $T = 300$ K

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

Temperature $T = 1500$ K

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
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Bibliography I


Bibliography II


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

$T = 1770.15 \text{ K, } x_{\text{H}_2\text{O}} = 0.9811, P_t = 1.0262 \text{ atm, } L = 54.00 \text{ cm, Voigt Lineshape}$

See also Ref. [3]