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

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Line-by-Line Method

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

- 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

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

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

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

\[
\varepsilon^{\text{tot}} = \frac{1}{\sigma \cdot T^4} \cdot \int_0^\infty \varepsilon \eta \cdot \frac{c_1 \cdot \eta^3}{\exp \left( \frac{c_2 \cdot \eta}{T} \right) - 1} \cdot d\eta
\]
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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)

CO₂ at 1770 K, \( x_{CO₂} = 0.43 \), \( x_{N₂} = 0.57 \), \( P_t = 1 \text{ atm} \), \( L = 54 \text{ cm} \)

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

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

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

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

see Alberti et. al. [3]
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

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

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

CO₂ Emissivity Chart, \( x_{CO₂} = x_{N₂} = 0.5 \)

\[ pL = p_{CO₂} \cdot L \]
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)
CO₂ / H₂O Emissivity Chart

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

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

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

- 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, 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)

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Taken from Hartmann [9]
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

Adjustments for Lorentz / Voigt Lineshape
High Pressure - Alberti et. al. (2015)

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

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 $\tau$

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

Temperature $T = 300$ K

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
  - CO\(_2\): maximum 2% difference (up to 1770 K)
  - H\(_2\)O: maximum 9% difference (up to 1770 K)
  - CO\(_2\) + H\(_2\)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


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

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

See also Ref. [3]
$T = 1770.15 \text{ K}, \ x_{\text{H}_2\text{O}} = 0.9811, \ P_t = 1.0262 \text{ atm}, \ L = 54.00 \text{ cm}, \ Voigt \ Lineshape$

See also Ref. [3]