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

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

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

\[ \varepsilon_{\text{tot}} = \frac{1}{\sigma \cdot T^4} \cdot \int_{0}^{\infty} \varepsilon_{\eta} \cdot \frac{c_1 \cdot \eta^3}{\exp \left( \frac{c_2 \cdot \eta}{T} \right) - 1} \cdot d\eta \]

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

Transmissivity \( \tau_{\eta} \)

\( \varepsilon_{\text{tot}} = 1800 \text{ K}, \ P_t = 1 \text{ atm}, \text{ pure H}_2\text{O}, \ L = 50 \text{ cm} \)
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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)

CO₂ at 1770 K, \( x_{CO_2} = 0.43, \ x_{N_2} = 0.57, \ P_t = 1 \ atm, \ L = 54 \ cm \)

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

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

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

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

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

H₂O and CO₂ at 1770 K, \( x_{\text{H}_2\text{O}} = x_{\text{CO}_2} = 0.43 \), \( P_t = 1 \text{ atm} \), \( L = 54 \text{ cm} \)

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

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

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

$\text{Total Emissivity}$

$\text{Temperature in K}$

$\text{Calculated using HITEMP-2010}$

$\times$ $\text{Calculated using Measurements of Alberti et. al. (2015)}$

$pL = p_{CO₂} \cdot L$
High Temperature - Alberti et. al. (2015)

H$_2$O Emissivity Chart, $x_{H_2O} = x_{N_2} = 0.5$

Temperature in K

Total Emissivity

10 bar cm
25 bar cm
55 bar cm

$pL = p_{H_2O} \cdot L$

Calculated using HITEMP-2010

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

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

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

- 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 $\tau$  

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

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

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

Temperature \( T = 300 \text{ K} \)

Total Emissivity

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
  - CO₂: maximum 2% difference (up to 1770 K)
  - H₂O: maximum 9% difference (up to 1770 K)
  - CO₂ + H₂O: 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


Bibliography II


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

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

\[
\frac{\tau_{\text{Lorentz}} - \tau_{\text{Voigt}}}{\tau_{\text{Voigt}}} \cdot 100 \%
\]

Wavenumber in cm\(^{-1}\)

See also Ref. [3]