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

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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

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

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

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

CO₂ at 1770 K, \(x_{\text{CO}_2} = 0.43, x_{\text{N}_2} = 0.57, P_t = 1 \text{ atm}, L = 54 \text{ cm}\)

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

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

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

\[
\text{Transmissivity } \tau \eta, \text{Measured} - \tau \eta, \text{HITEMP-2010}
\]

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

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

Temperature in K

Total Emissivity

$pL = p_{CO₂} \cdot L$

Calculated using HITEMP-2010

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

H₂O Emissivity Chart, \( x_{H_2O} = x_{N_2} = 0.5 \)

\[
pL = p_{H2O} \cdot L
\]

Calculated using HITEMP-2010

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

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

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

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

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

\[ pL = (p_{CO_2} + p_{H_2O}) \cdot L \]
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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 $\tau$  = 303 K, $P_t$ = 11.1 bar, pure CO$_2$, $L$ = 5.02 cm

Fukabori (1986) No Limit Limited (60 $\Delta$) $\chi$-Tran (2011) ······ FLM

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

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

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

Temperature $T = 300$ K

Total pressure in bar

Total Emissivity

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

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

Temperature $T = 1500$ K

Total pressure in bar

Total Emissivity

- 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

\[
\tau_\eta = \frac{(I_{\text{hot}N_2} - I_{\text{cold}N_2})}{(I_{\text{hot}\text{gas}} - I_{\text{cold}\text{gas}})}
\]
$T = 1770.15\,\text{K}$, $x_{\text{H}_2\text{O}} = 0.9811$, $P_t = 1.0262\,\text{atm}$, $L = 54.00\,\text{cm}$, Voigt Lineshape

See also Ref. [3]