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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5 – 9 July, 2015
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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

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

\[ \varepsilon_\eta = 1 - \tau_\eta \]

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

CO\(_2\) 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

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

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

H\textsubscript{2}O and CO\textsubscript{2} at 1770 K, x\textsubscript{H\textsubscript{2}O} = x\textsubscript{CO\textsubscript{2}} = 0.43, P\textsubscript{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)

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

- $pL = p_{CO_2} \cdot L$

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

- 9 bar cm
- 24 bar cm
- 38 bar cm
- 55 bar cm

Temperature in K

Total Emissivity
High Temperature - Alberti et. al. (2015)

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

$\rho L = \rho_{H2O} \cdot L$

Calculated using HITEMP-2010

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

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

\[
P_{H_2O} \quad \frac{p_{H_2O}}{p_{CO_2}} = 1.0, \quad 4.0, \quad 0.25
\]

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

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

[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
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 \( \tau \eta \)

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

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

Temperature $T = 300$ 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

The authors gratefully acknowledge the financial support by the Helmholtz Association of German Research Centres (HGF) in the frame of the Helmholtz Virtual Institute for Gasification Technology - HVIGasTech (VH-VI-429).
Bibliography I


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

See also Ref. [3]