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

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Publication date: 2015

Document Version
Peer reviewed version

Citation (APA):
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10th International Conference on Industrial Furnaces and Boilers

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April 9, 2015
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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

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

\[ T = 1800 \, \text{K}, \quad P_t = 1 \, \text{atm}, \quad \text{pure CO}_2, \quad L = 50 \, \text{cm} \]
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, 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\(^{-1}\)
CO$_2$ at 1770 K, $x_{CO_2} = 0.43$, $x_{N_2} = 0.57$, $P_t = 1$ 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)

\[ \text{H}_2\text{O at 1770 K, } x_{\text{H}_2\text{O}} = 0.43, x_{\text{N}_2} = 0.57, P_t = 1 \text{ atm, } L = 54 \text{ cm} \]

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

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

H$_2$O 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, $x_{CO₂} = x_{N₂} = 0.5$

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

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

H$_2$O Emissivity Chart, $x_{\text{H}_2\text{O}} = x_{\text{N}_2} = 0.5$

$pL = p_{\text{H}_2\text{O}} \cdot L$

Calculated using HITEMP-2010

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

$CO_2 / H_2O$ Emissivity Chart

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

$\frac{p_{H_2O}}{p_{CO_2}} = 4.0$

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

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, 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)

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

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

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

Transmissivity $\tau$

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

Temperature $T = 300$ K

<table>
<thead>
<tr>
<th>Total pressure in bar</th>
<th>Total Emissivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 bar cm</td>
<td>0.10</td>
</tr>
<tr>
<td>500 bar cm</td>
<td>0.20</td>
</tr>
<tr>
<td>80 bar cm</td>
<td>0.30</td>
</tr>
</tbody>
</table>

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
  - 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


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

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

See also Ref. [3]