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
Contents

Line-by-Line Method

High Temperature

High Pressure

Summary and Conclusion
Content of this Chapter

Line-by-Line Method

High Temperature

High Pressure

Summary and Conclusion
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

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

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

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

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

Line-by-Line Method

High Temperature

High Pressure

Summary and Conclusion
High Temperature

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)

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

Transmissivity $\tau_\eta$

Difference

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)

$H_2O$ and $CO_2$ at 1770 K, $x_{H_2O} = x_{CO_2} = 0.43$, $P_t = 1$ 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)

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)

$H_2O$ 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)
High Temperature - Alberti et. al. (2015)

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

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

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

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

\[ \text{Temperature in K} \]

\[ \text{Total Emissivity} \]

\[ \text{Calculated using HITEMP-2010} \]

\[ \times \text{Calculated using Measurements of Alberti et. al. (2015)} \]
Content of this Chapter

Line-by-Line Method

High Temperature

High Pressure

Summary and Conclusion
High Pressure

Important Results for CO₂ (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]
    - 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 \( \tau \eta \)

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 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]
Content of this Chapter

Line-by-Line Method

High Temperature

High Pressure

Summary and Conclusion
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
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


Bibliography II


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]