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On the accuracy of HITEMP-2010 calculated emissivities of water vapor and carbon dioxide

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Line-by-Line Method

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Summary and Conclusion
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

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

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

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

$$\varepsilon^{\text{tot}} = \frac{1}{\sigma \cdot T^4} \int_0^\infty \varepsilon \eta \cdot \frac{c_1 \cdot \eta^3}{\exp \left( \frac{c_2 \cdot \eta}{T} \right) - 1} \cdot d\eta$$
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High Temperature

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)

CO₂ at 1770 K, \( x_{CO₂} = 0.43 \), \( x_{N₂} = 0.57 \), \( P_t = 1 \) 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)

H₂O 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)

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

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

\[ pL = p_{H_2O} \cdot L \]
High Temperature - Alberti et. al. (2015)

\[
(p_{\text{CO}_2} + p_{\text{H}_2\text{O}}) \cdot L = 47 \text{ bar cm}
\]

\[
p_{\text{H}_2\text{O}} / p_{\text{CO}_2} = 4.0
\]

\[
p_{\text{H}_2\text{O}} / p_{\text{CO}_2} = 1.0
\]

\[
p_{\text{H}_2\text{O}} / p_{\text{CO}_2} = 0.25
\]

\[
\begin{align*}
\text{Total Emissivity} & \quad \text{Temperature in K} \\
0.40 & \quad 400 \\
0.30 & \quad 600 \\
0.20 & \quad 800 \\
0.10 & \quad 1000 \\
\end{align*}
\]

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

\[
pL = (p_{\text{CO}_2} + p_{\text{H}_2\text{O}}) \cdot L
\]
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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**
  - 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 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**
  
  Line-Mixing (finite duration of collision)

![Graph of absorption over wavenumber](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)

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

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 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


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

See also Ref. [3]