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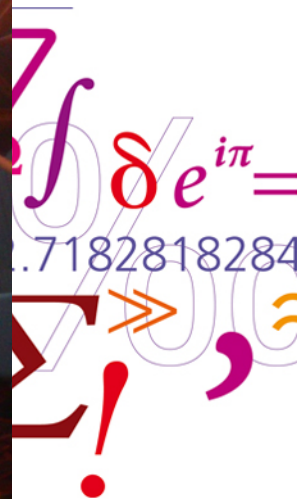
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High-resolution spectroscopy of gases at elevated temperatures for industrial applications

Alexander Fateev and Sønnik Clausen

Optical Diagnostics Group,

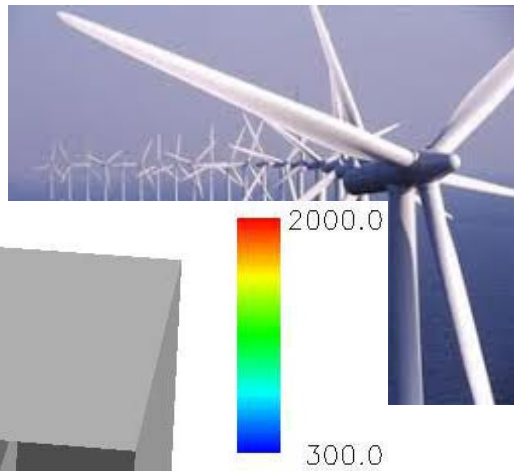
DTU Chemical Engineering, Frederiksborgvej 399, Roskilde, DK-4000, Denmark



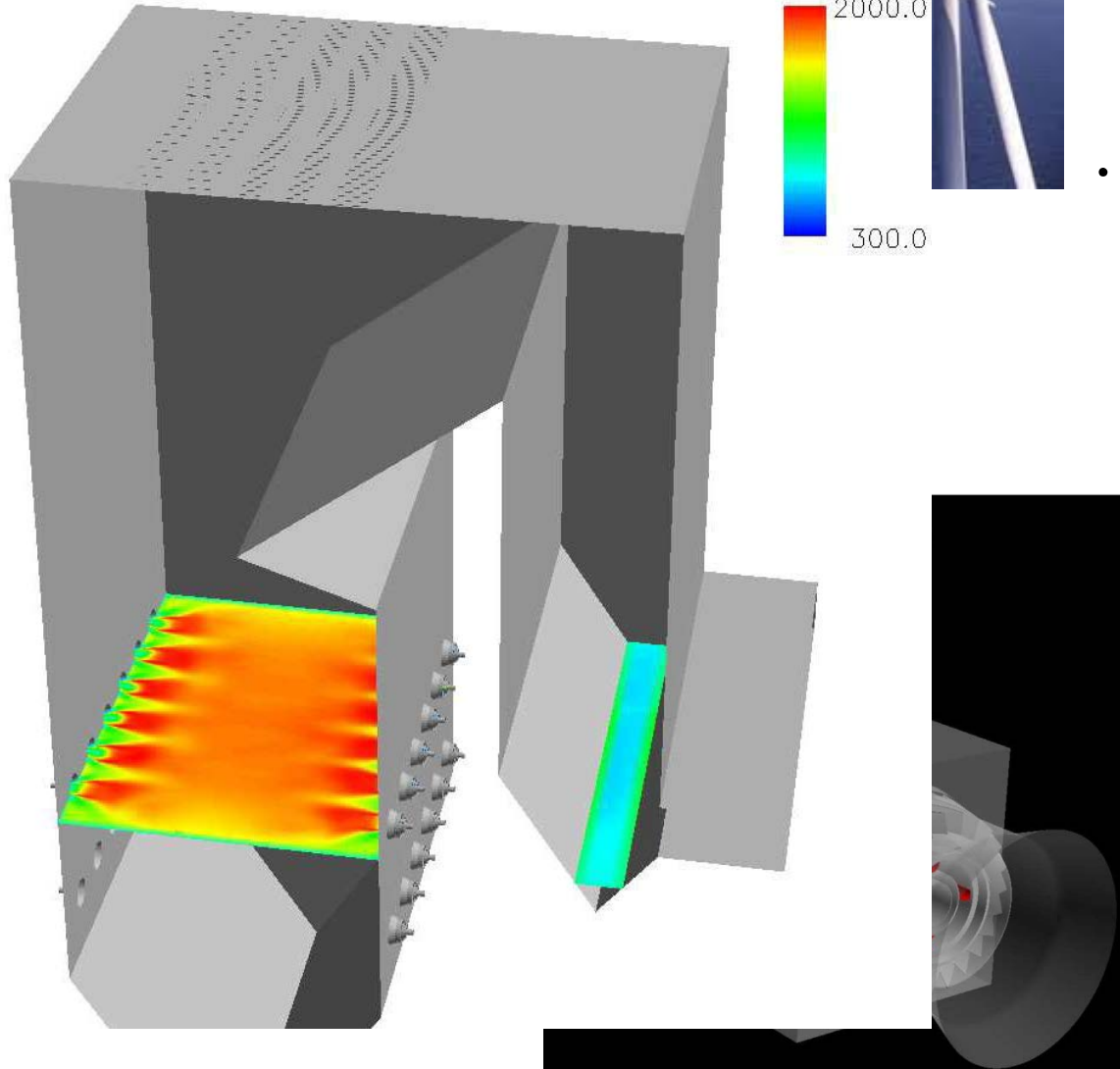
Outline

- Large scale measurements: why?
- Basic research: how it's made
- High resolution spectroscopy in flow gas cells: H₂O and CO₂
- SO₃ project: the story
- Conclusions

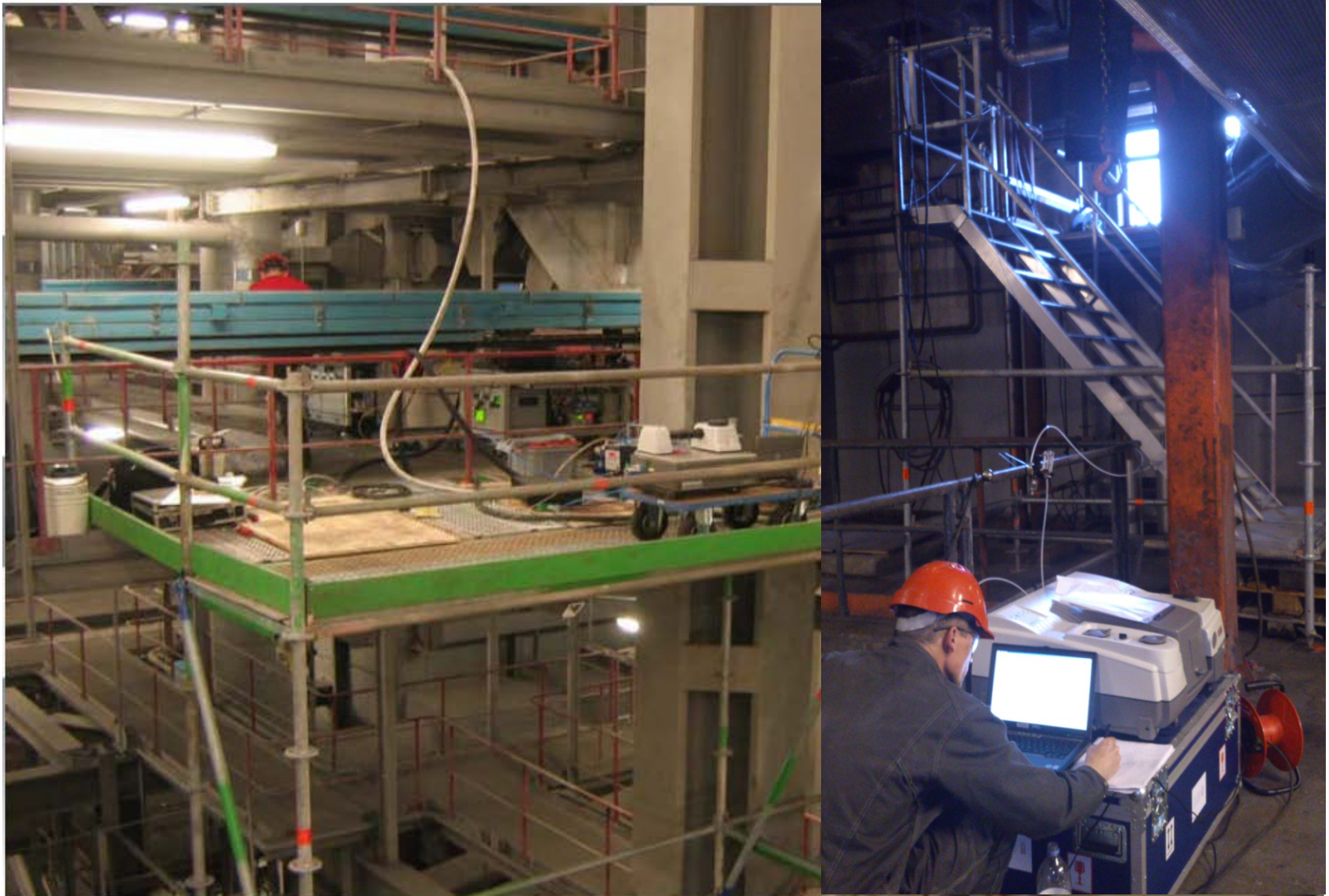
Green Energy...



... well



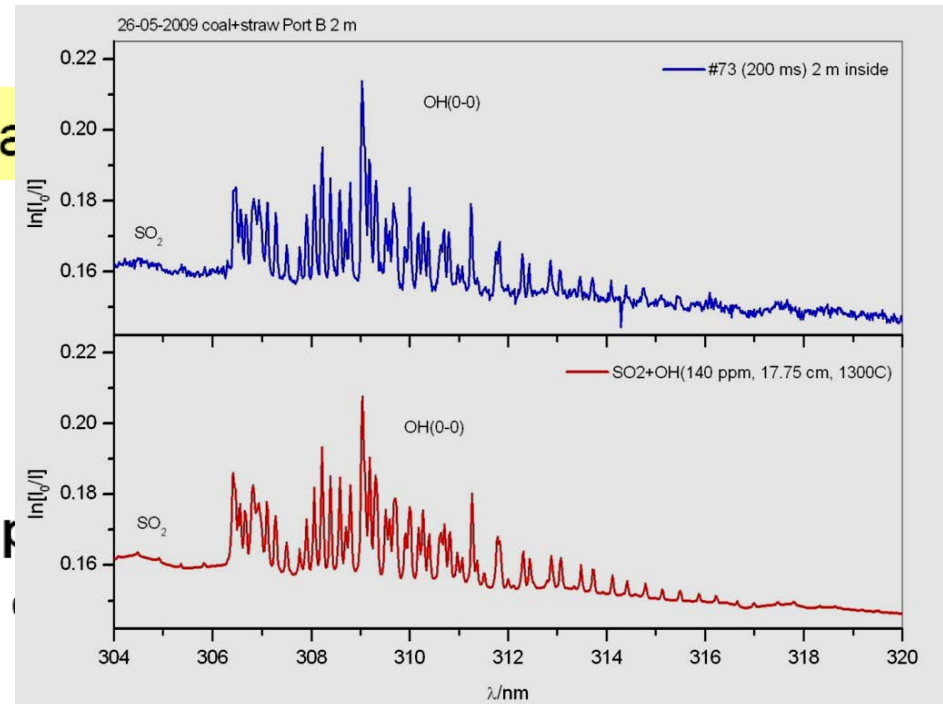
Large scale measurements



Large scale measurements

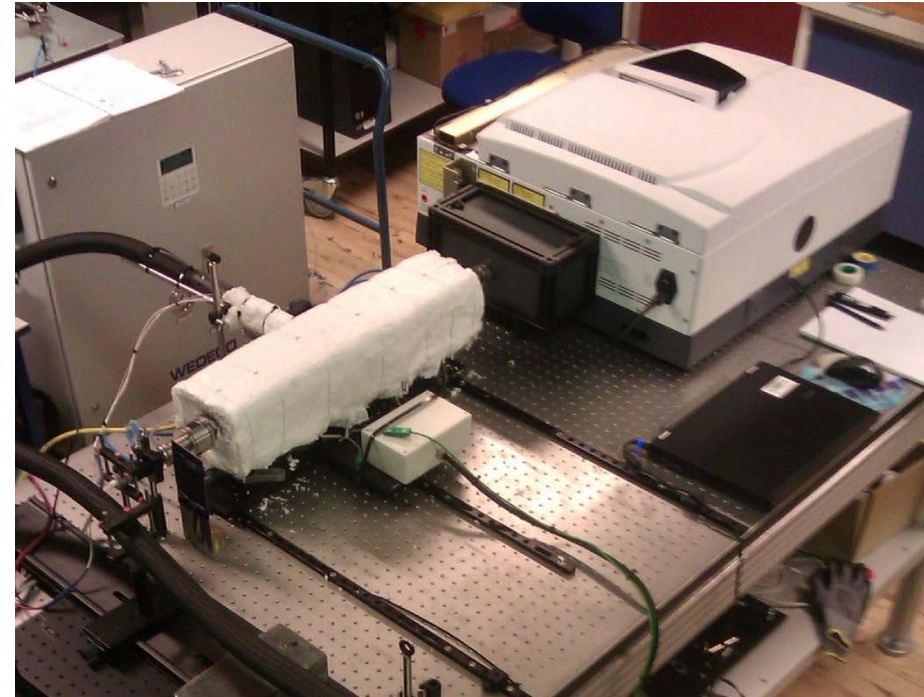
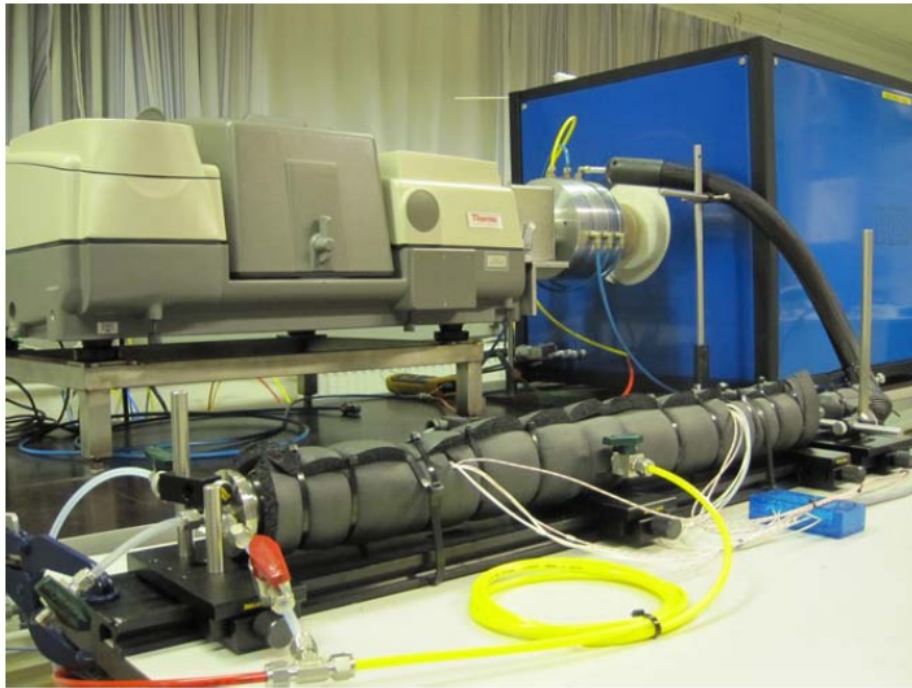
Fiber optical probes

- FTIR spectroscopy (emission): >5 m, 45 mm probe
 H_2O , CO_2 , CO , C_xH_y , HCl , etc. + T_{gas} + T_{par} + ϵ
- UV spectroscopy (transmission): 9 m, 60 mm probe
 SO_2 , NO , O_2 , etc.



Basic research

- focus on optical properties (TRS, ABS) of gases at temperatures up to 1600C;
- validation/building databases (e.g. HITRAN/HITEMP/CDSD...);
- high-resolution spectroscopy (0.125 cm⁻¹/0.016 nm) of “major” and “minor” (or trace) gases : CO₂, H₂O, SO₂, NH₃, SO₃, H₂S, OCS, HCL, CH₃Cl, PAH's etc;
- various hot gas cells with highly-uniform temperature profiles (± 0.5 C).

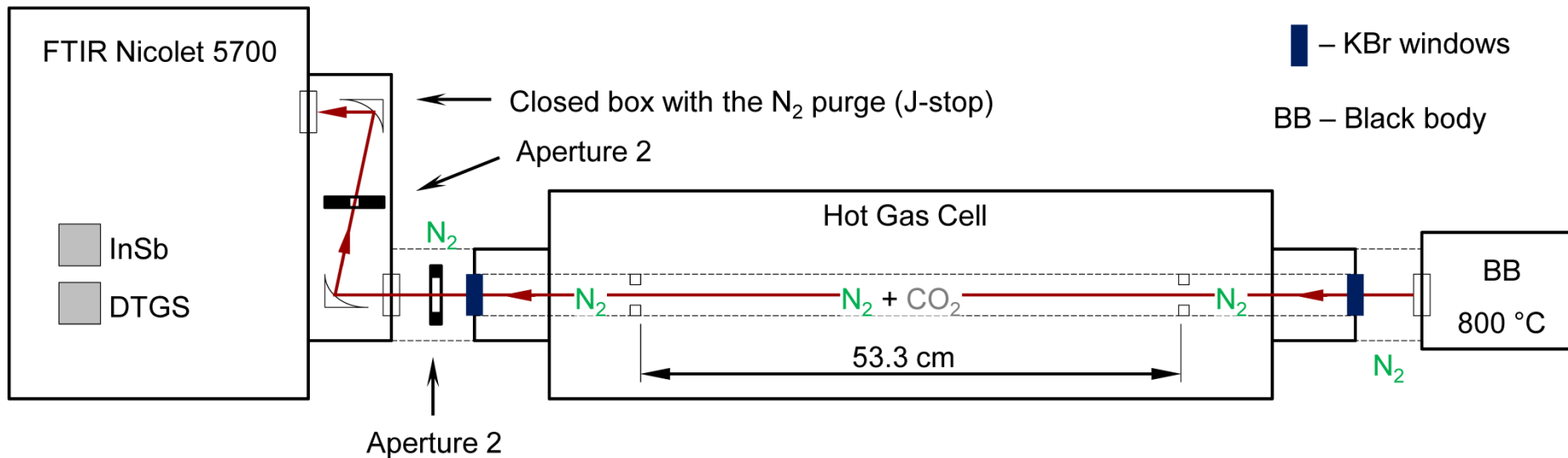


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Experimental set up

Includes:

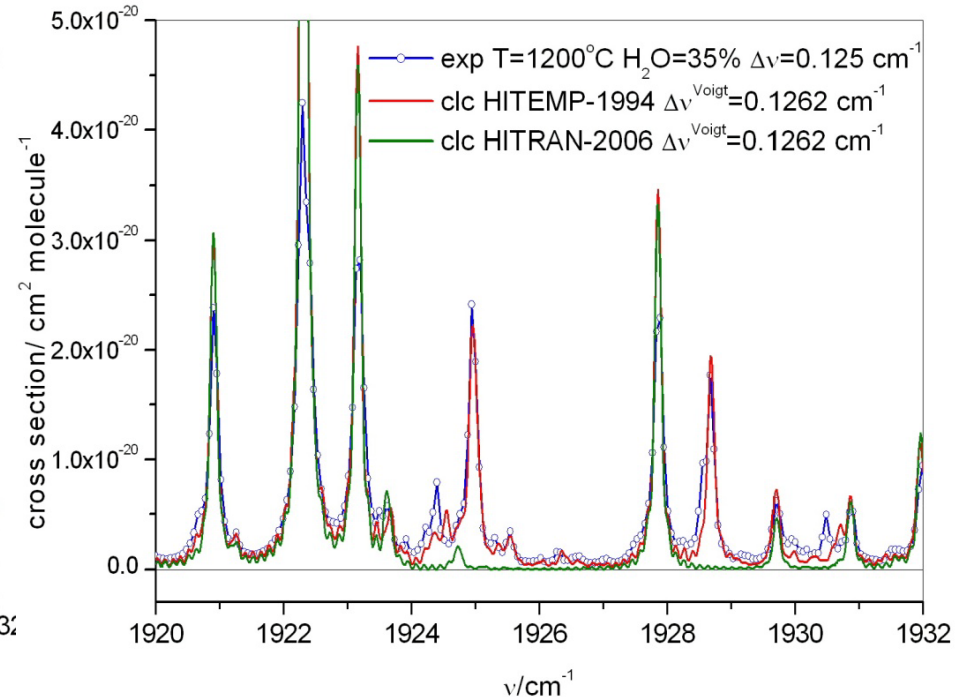
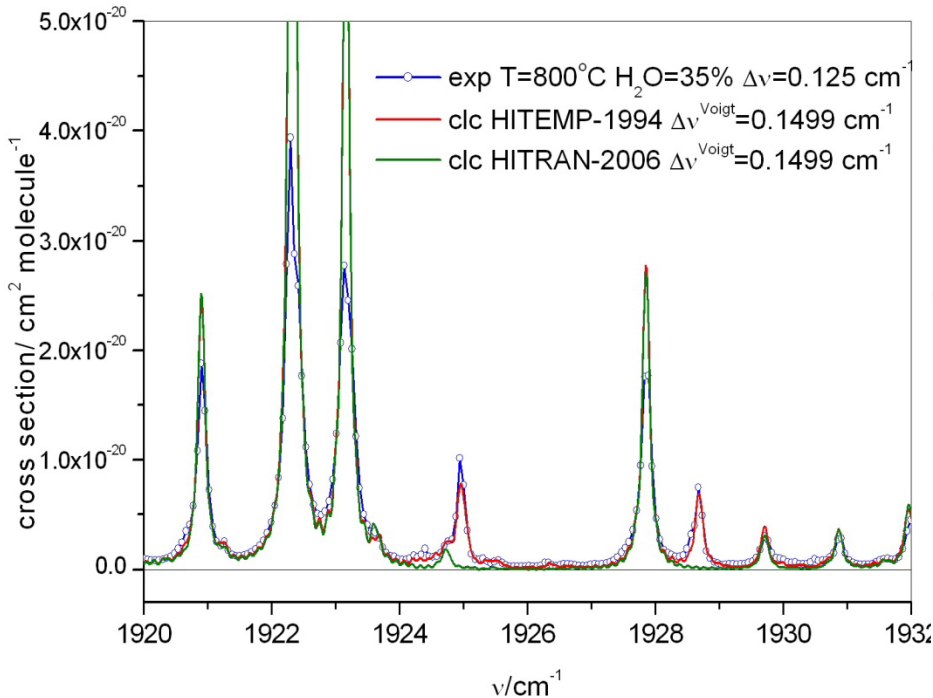
- a gas cell;
- a high-resolution FTIR spectrometer (Nicolet or Agilent);
- a light source (BB).



Examples: H2O absorption cross sections

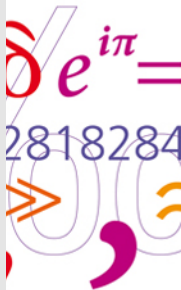
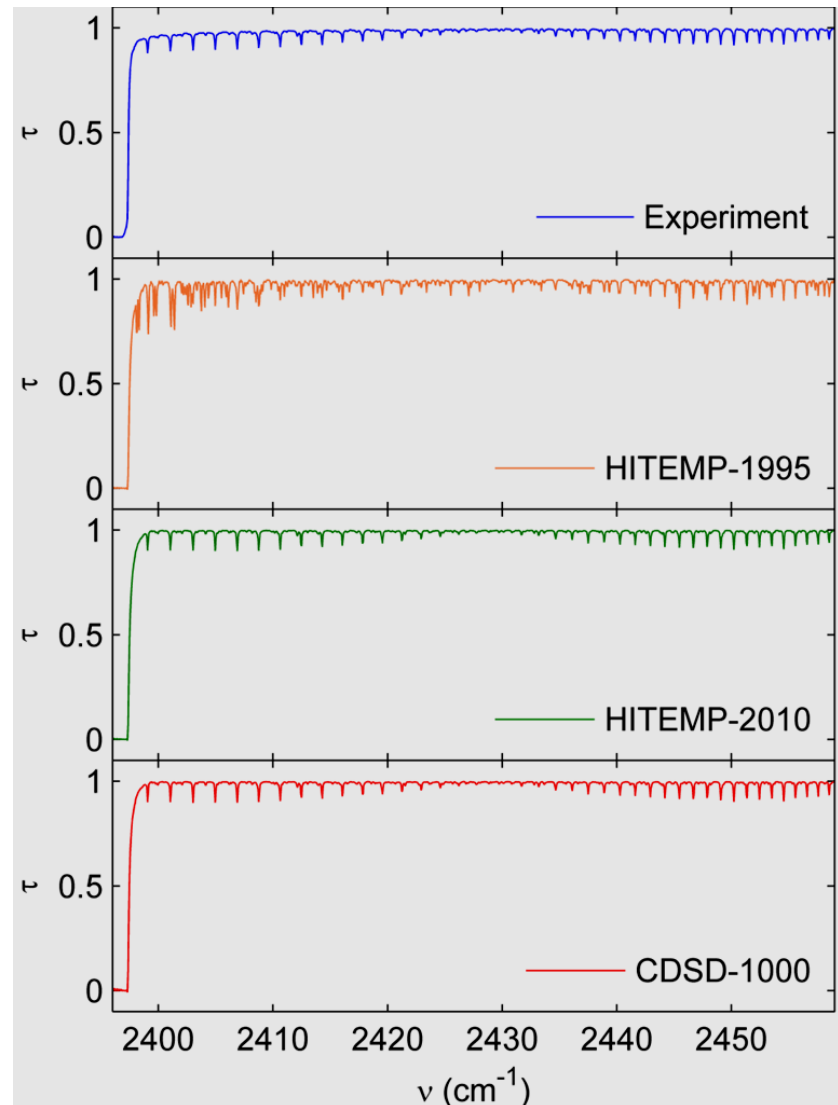
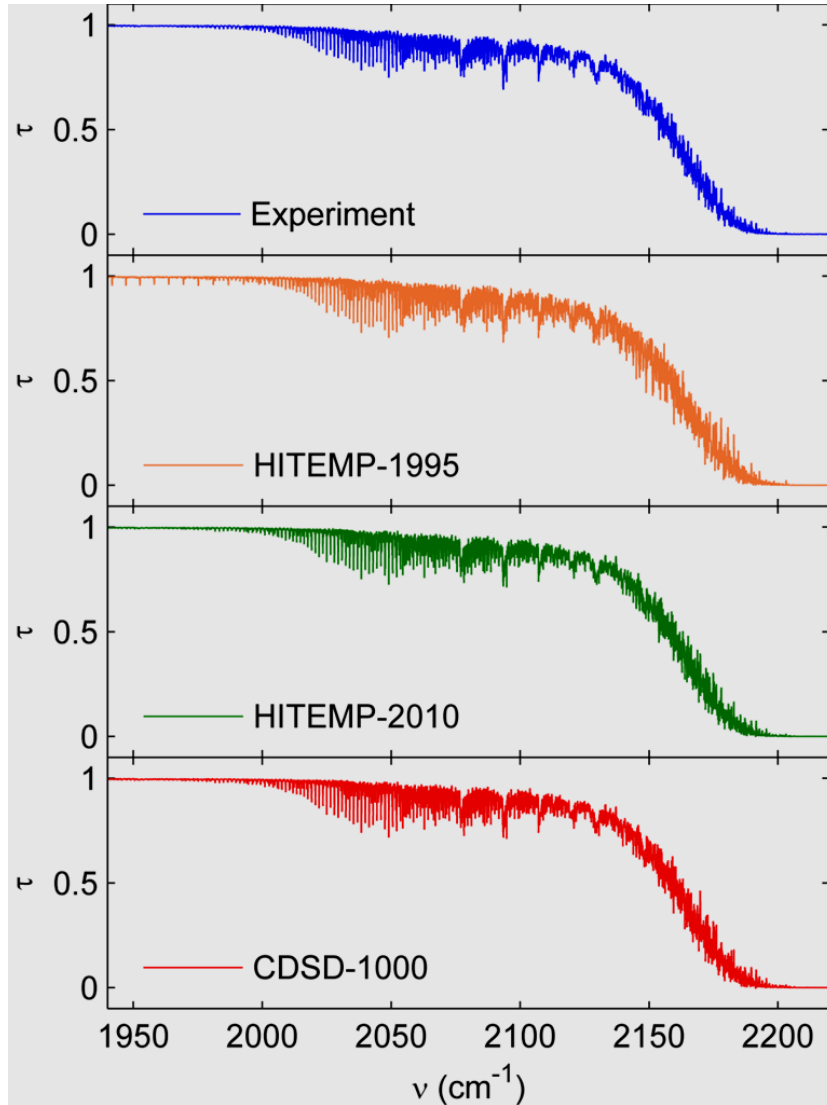
T=800C

T=1200C

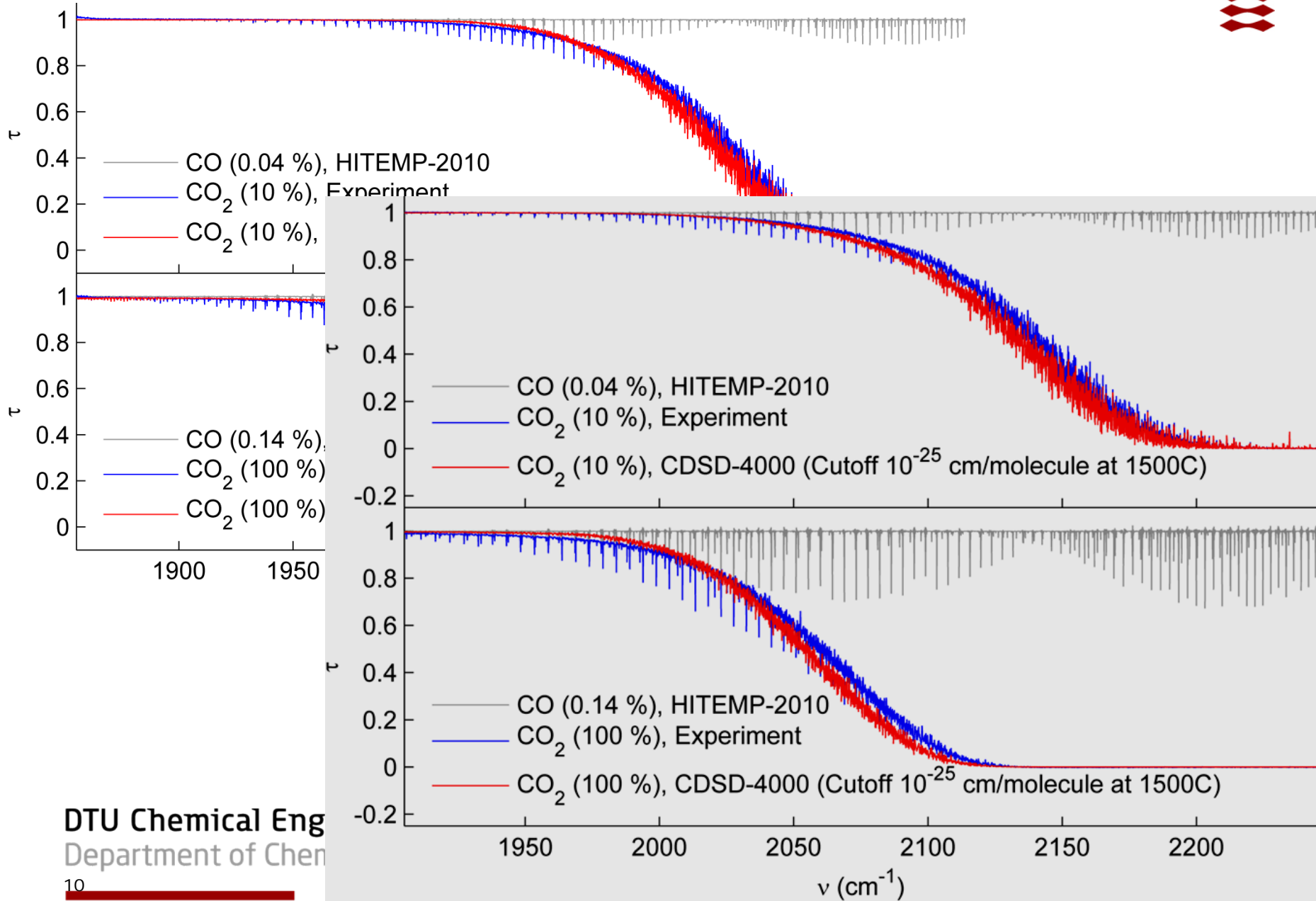


- Good agreement between EXP and CLC(HITEMP-1994);
- Different FWHM values of the H₂O single lines for H₂O(35%) in N₂ and H₂O(35%) in CO₂ (oxyfuel combustion).

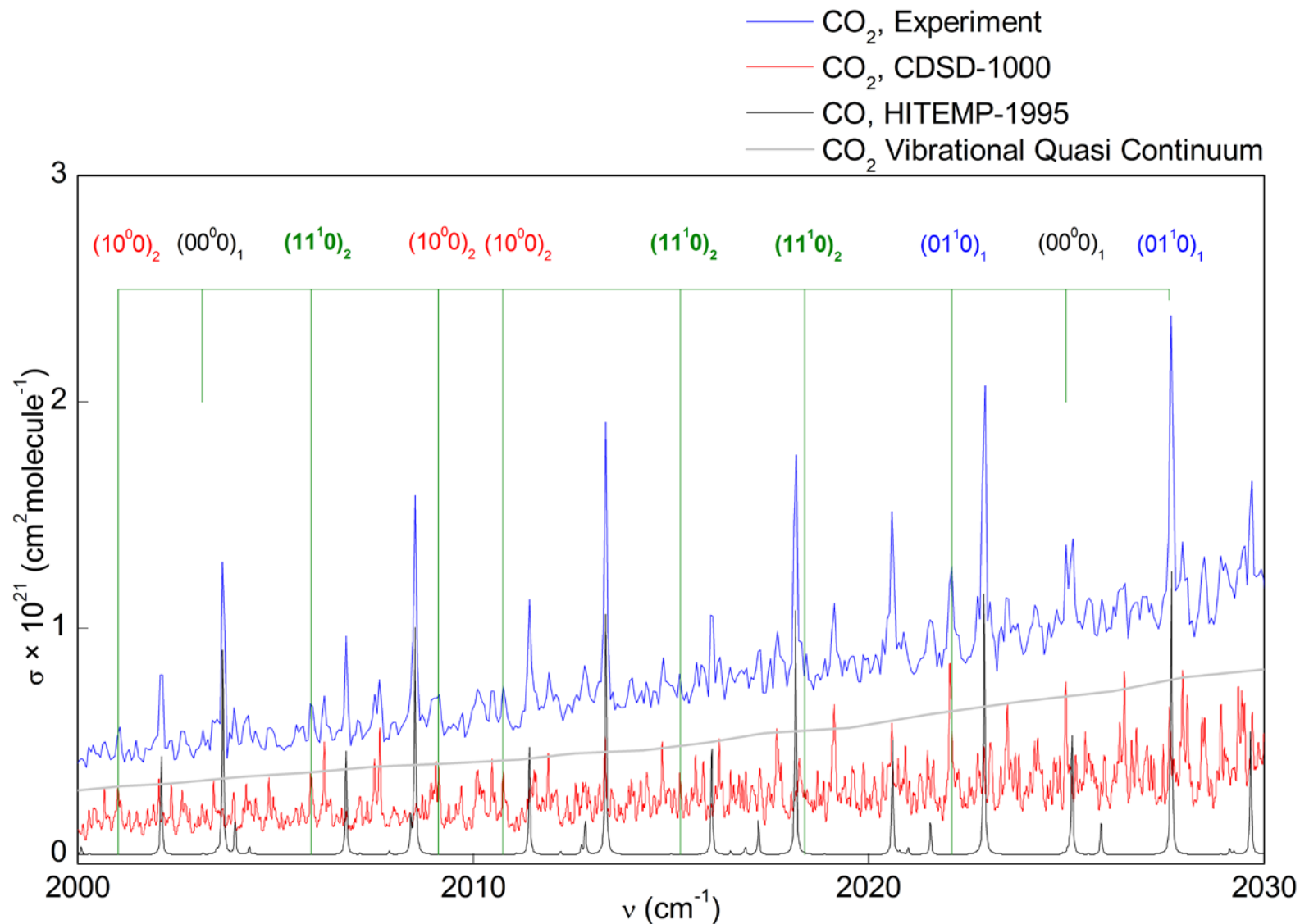
CO2 transmission spectra: 727C



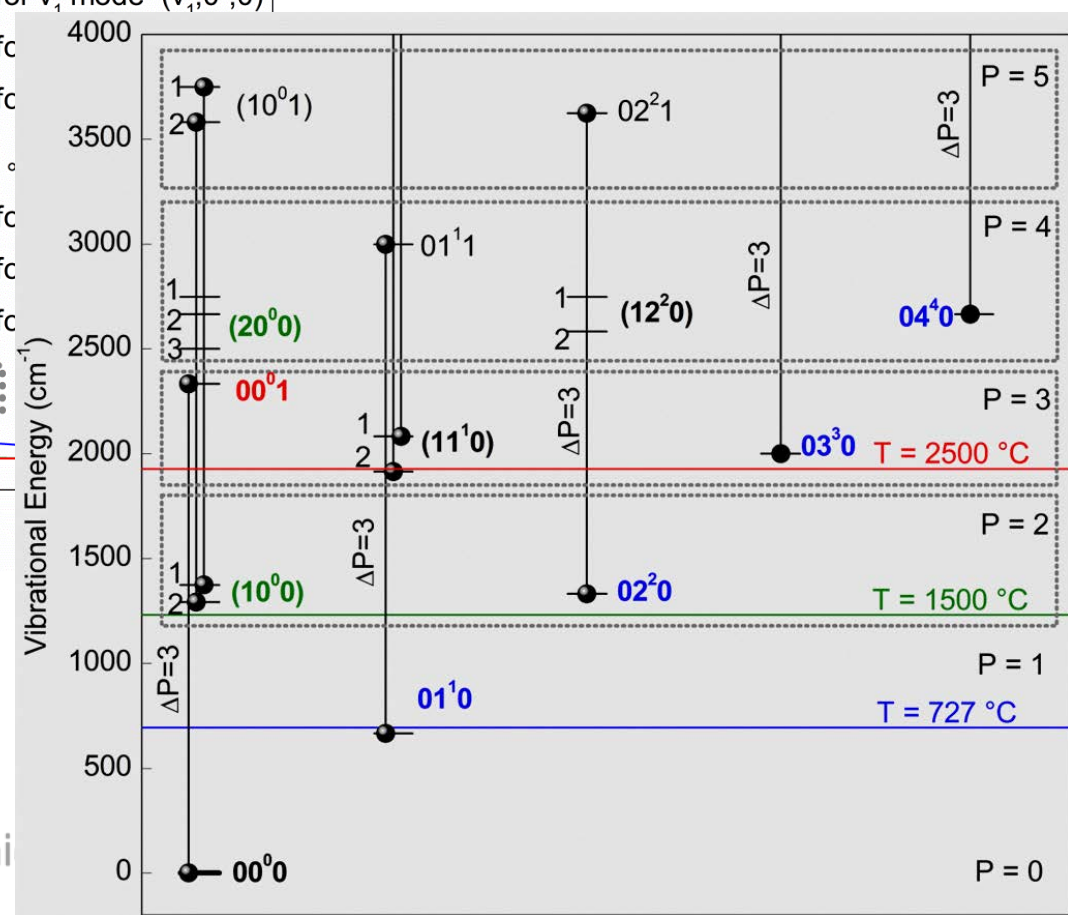
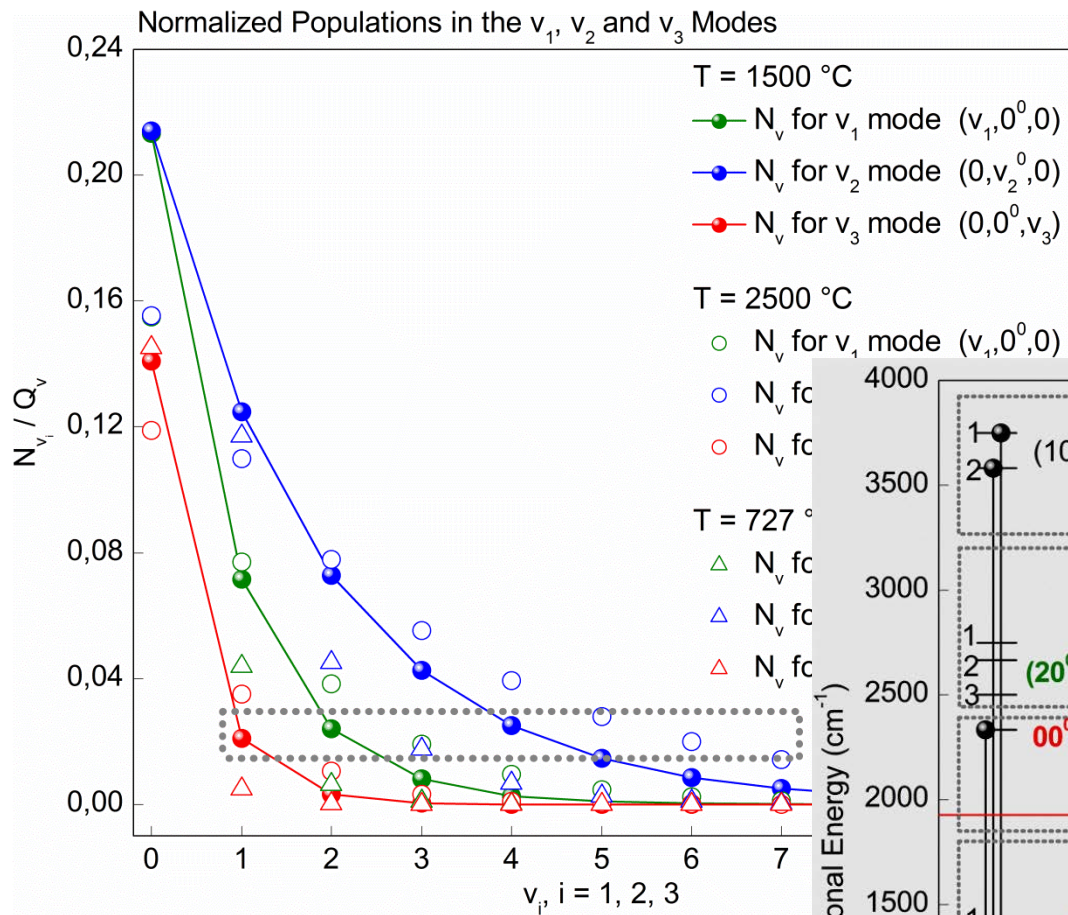
CO2 transmission spectra: 1500C



CO₂ quasicontinuum at 1500C



CO2 quasicontinuum at 1500C



SO3 project: industry and university



Facts:

- Coal air combustion: SO₂(300ppm) and SO₃(5ppm) (blue smog);
- Large power plants: SCR units (NO_x reduction) with NH₃ injection;
- Global warming: operation at lower loads;
- Lower loads: lower gas temperatures at SCR units;
- By law: not allowed to turn off NH₃ injection system.

Problems:

- Non optimal NH₃ consumption;
- At lower T: H₂SO₄ formation which causes ammonia sulfate and ammonia bisulfate formation;

Consequences:

corrosion in ducts and plugging/damage of SCR elements.

Goal:

to develop an optical method for SO₃ *in situ* measurements.

SO3 project: industry and university

Challenges of the project:

- temperature range 200-500C;
- SO3 high-resolution spectra (SO3 generation);
- SO2, NH3, H2SO4 and H2O high-resolution spectra database;

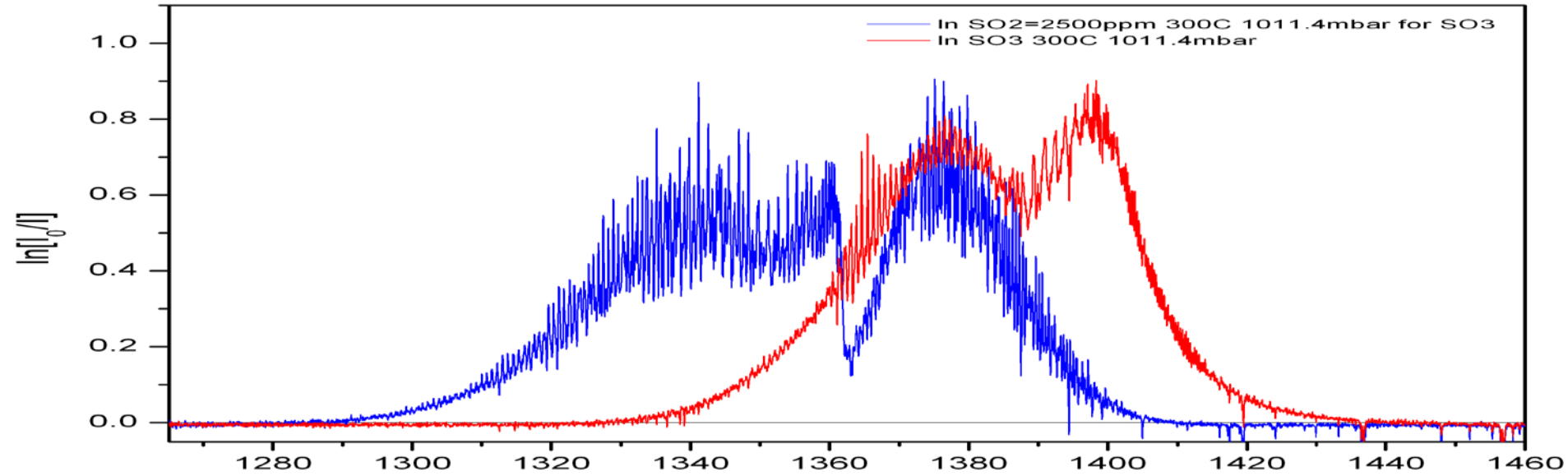
- water cooled optical probe development;
- powerful IR light source development;
- high sensitivity FTIR with linearized MCT or InSb detector;
- use of modern mathematical tools (e.g. SVD, NNLS).

Two phases of the project:

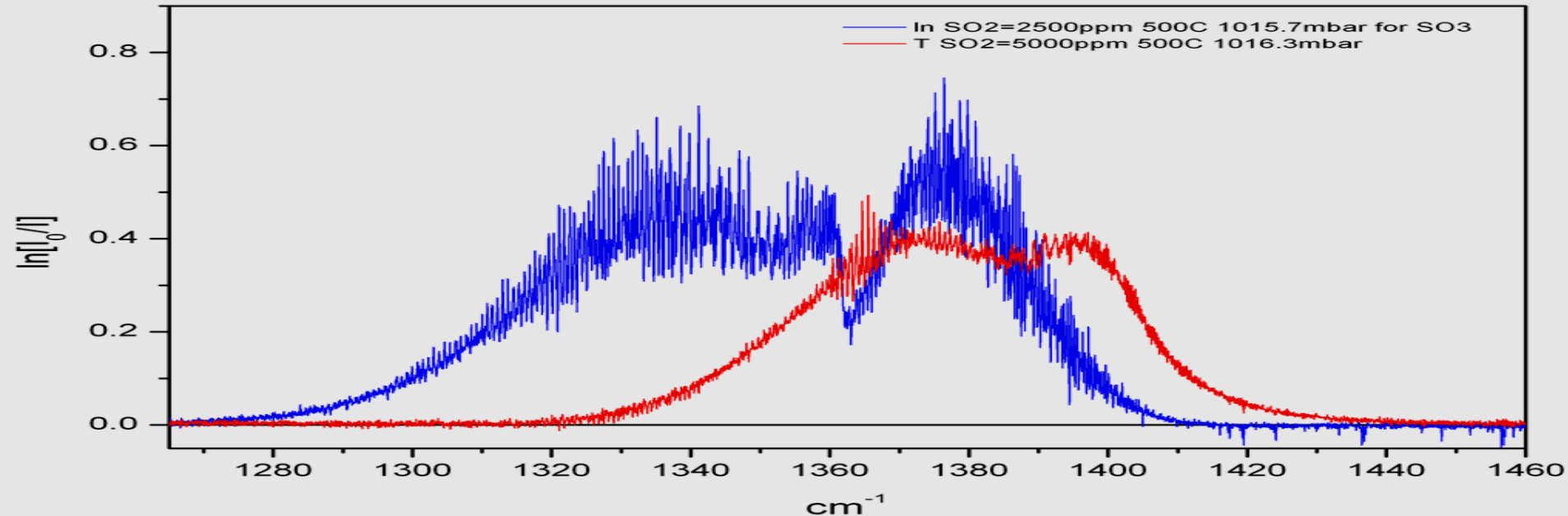
- measurements in the lab and SO2/SO3 line list generation (UCL, UK)
- measurements on an industrial scale (power plant, Dong Energy, DK)

SO3 project: high-resolution (0.115 cm⁻¹) measurements

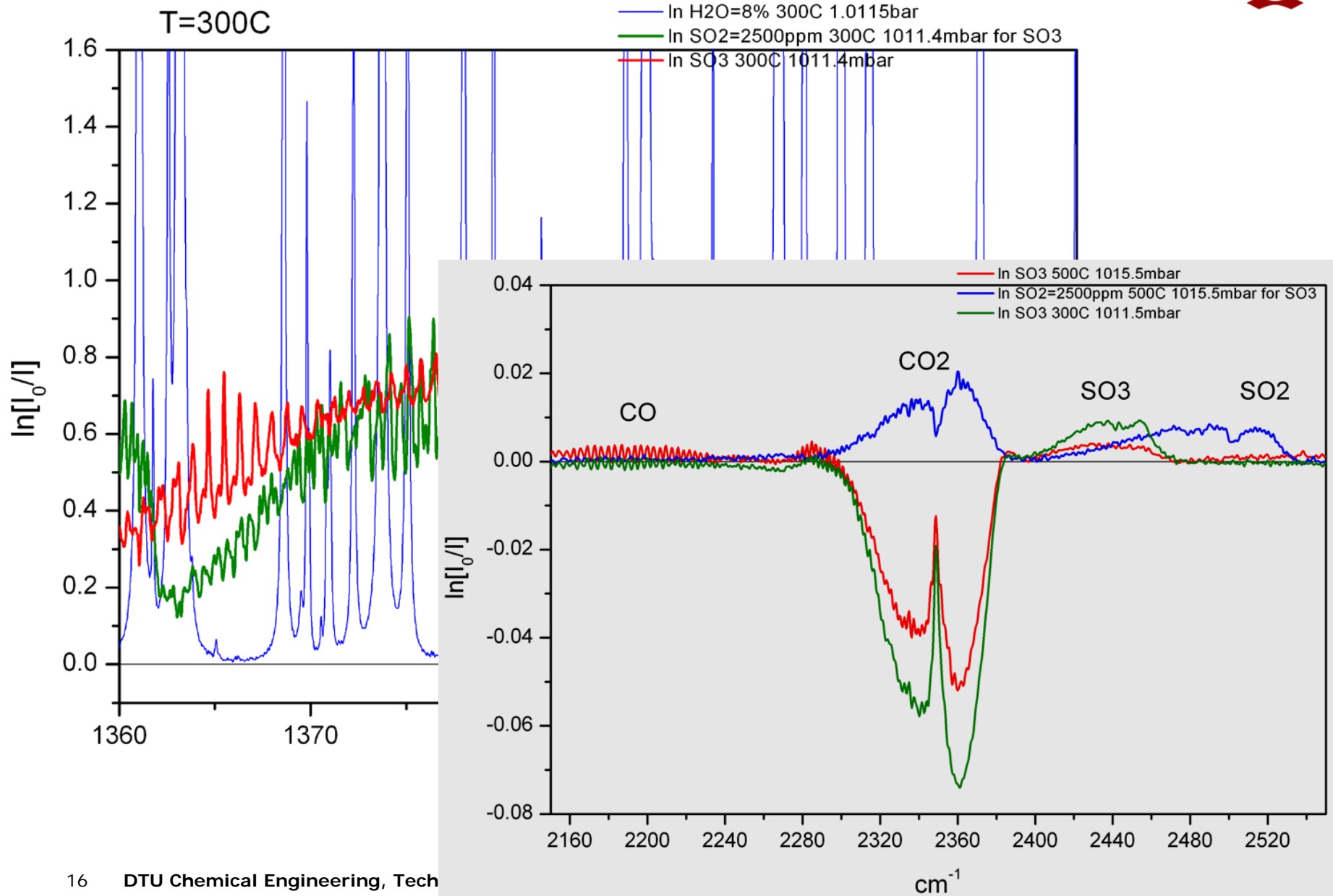
T=300C



T=500C



SO3 project: interferences



Conclusions

High quality optical measurements with various gases (incl. highly corrosive gases) are possible;

A new gas cell is under development (<200 bar, 2000C)

Measurements can be used for: databases development and validation, studies of chemical reactions, energy exchange, validation of line shape models.

SO₃ project is under development: lab work + PhD student employed by UCL;



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- UCL (Prof. Jonathan Tennyson)