Analyzing Molecular IR-Emission Spectra of Deflagrating Methane Air Mixtures at Different Pressures

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Key words

NIR-Emission spectroscopy, deflagration, molecular spectra

Abstract

Methane air mixtures at two different pressures (0.1 and 1 MPa) have been ignited in an high pressure vessel to study the emitted radiation in the near and mid infrared spectral range during the deflagration process. The gas temperature and the optical depth were determined by comparing the experimental molecular band spectra to calculated intensity distributions. The obtained results show that NIR-emission spectroscopy allows monitoring chemical and physical processes of propagating flame fronts.

Experimental

The experiments were done in an optical bomb, a high pressure vessel equipped with two opposite windows (maximum pressure 20 MPa) allowing a non-intrusive process monitoring applying optical flame diagnostics. The investigated methane air mixtures were ignited at two different pressures of 0.1 and 1 MPa. The emitted infrared radiation has been detected by using a Zeiss MCS 511 NIR spectrometer and a self-developed filter-wheel system for the mid infrared. The Zeiss MCS 511 is a grating spectrometer with a InGaAs diode array as detector (spectral range 0.9 to 1.7 micron). The spectral resolution is about 15 nm at a scan rate of 300 spectra per second. The mid infrared system uses rotating filter wheels as monochromator and allows the detection of 100 spectra per second in a spectral range from 2.4 to 14 microns with an average spectral resolution of 100 nm. To calibrate the spectrometer systems, a black body radiator was used.

Data Analysis

The modeling code of the infrared band spectra developed at ICT together with ‘wispro’ is based on the data published in the ‘Handbook of Infrared Radiation from Combustion Gases’. It allows the calculating the emission and transmission spectra of H_2O (1.3, 1.8, 2.7 and 6.2 µm), CO_2 (2.7 and 4.3 µm), CO (4.65 µm), NO (5.3 µm) and HCl (3.5 µm) in a temperature range from 600 to 3000 K taking into account self absorption, pressure broadening and soot. The calculated intensity distributions are compared to experimental spectra by a least-squares fit routine with the parameter temperature and concentration length. Examples for the data analysis are shown in figure 1 and 2.

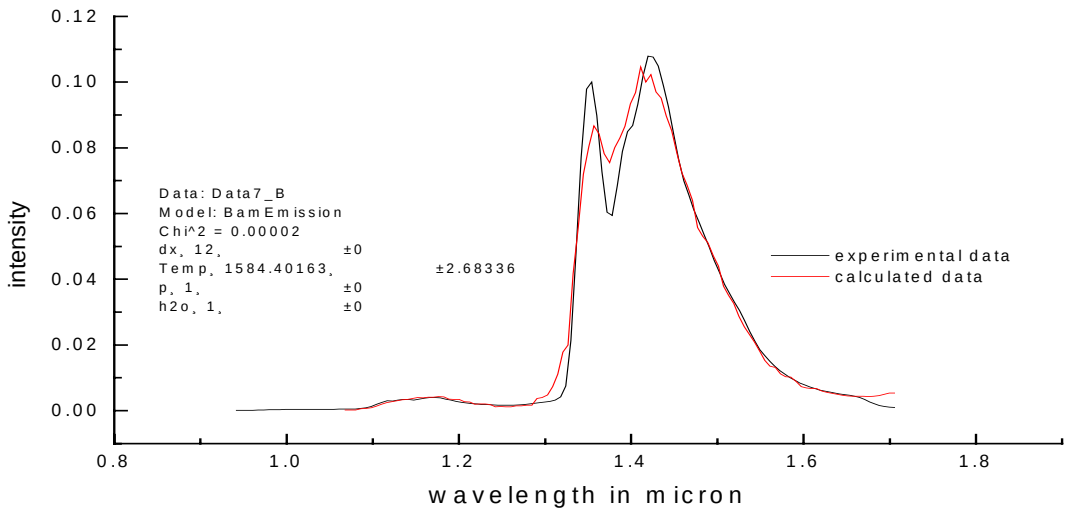

Fig.1: Comparison of an experimental and calculated NIR spectrum

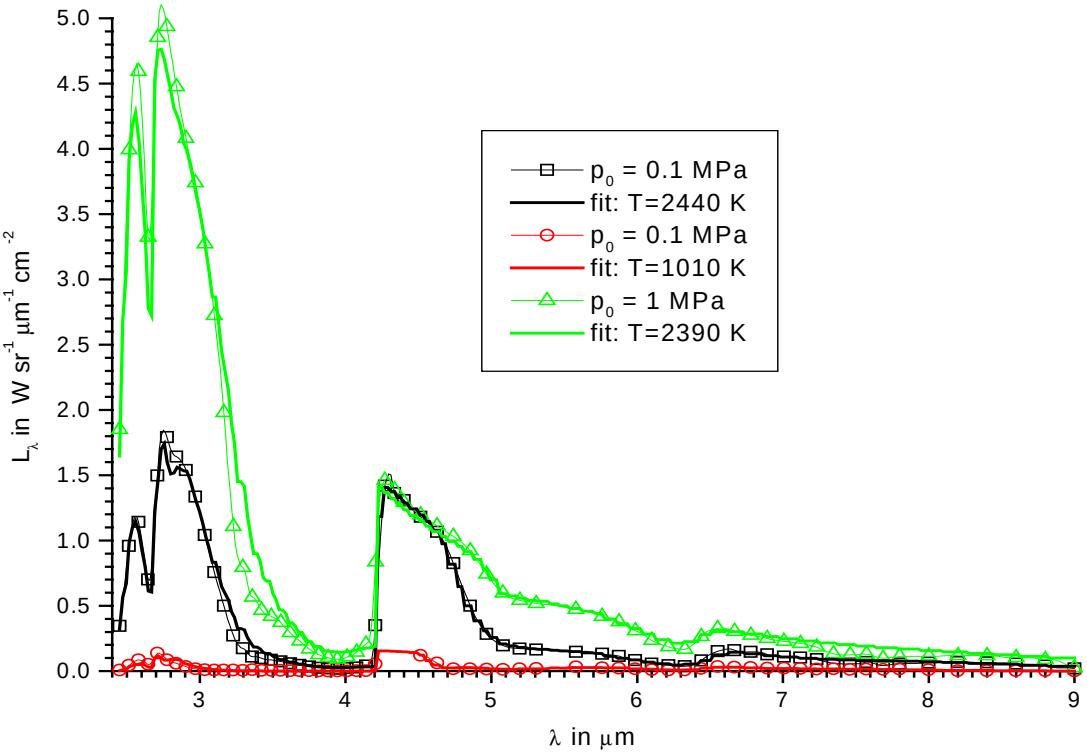

Fig. 2: Comparison of an experimental and calculated MIR spectrum

Results and Conclusions

The results show, that the sum of the optical depth of the C1 products in the wave front is approximately constant. CO as the intermediate combustion product disappears at the end of flame front while the end products water and carbon dioxide increase continuously. In the temperature progress, a decrease is observable, caused by heat radiation (see figure 3 and 4). The absolute temperature values seem to be a little high compared to themodynamical calculations.

But as a resume, the investigations showed, that NIR-emission spectroscopy allows monitoring chemical and physical processes of propagating flame fronts.

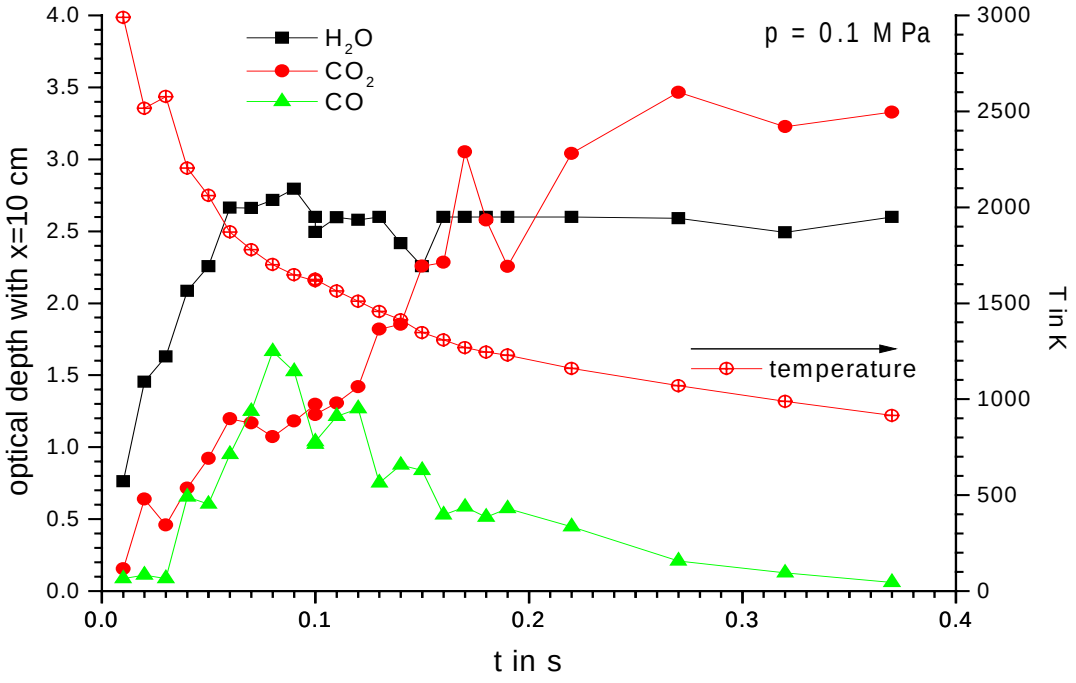

Fig. 3: Optical depth and temperature progress of the investigated methane air deflagrations at 0.1 MPa

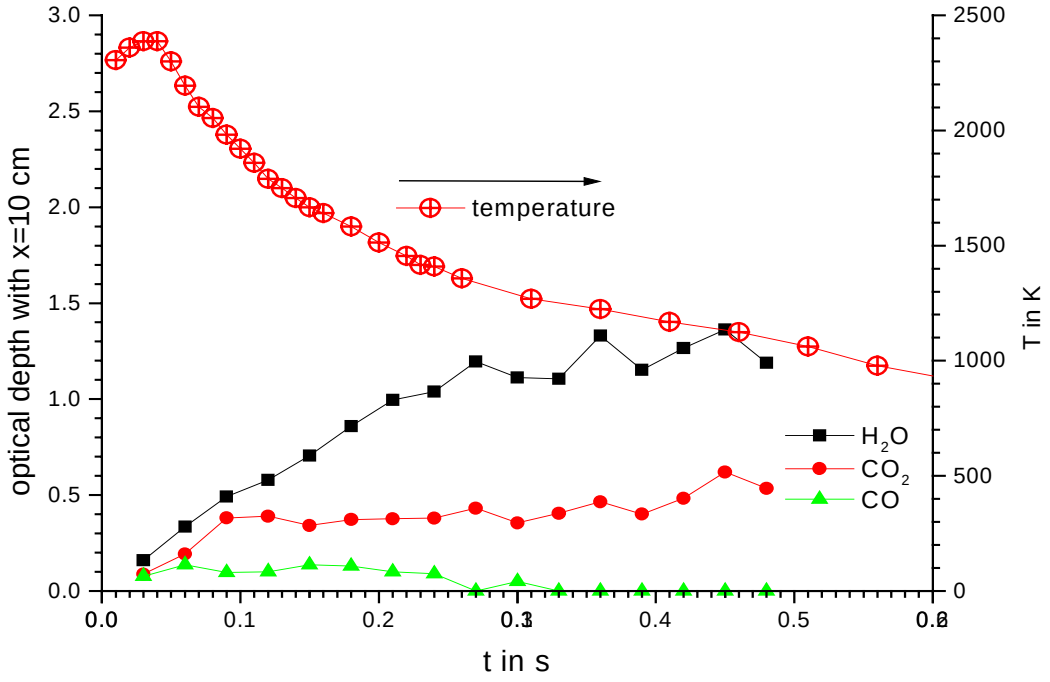

Fig. 4: Optical depth and temperature progress of the investigated methane air deflagrations at 1 MPa