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A METHOD FOR SPECTROSCOPIC TEMPERATURE MEASUREMENTS IN A SOLID FUEL COMBUSTION CHAMBER

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SUMMARY

In this report a simple spectroscopic method and spectroscopic setup, to determine flame temperatures $T$ in a Solid Fuel Combustion Chamber (SFCC), is described.

For an isothermal and well transparent flame, $T$ is calculated directly from the (constant) slope of a $\log f(E_j)$ versus $E_j$ graph, $f(E_j)$ being the (relative) occupation of the molecular energy level $E_j$.

If the slope turns out to be varying with $E_j$, a shell model for the flame must be applied to determine the temperature $T(r)$ as a function of the distance $r$ to the SFCC axis.

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1. INTRODUCTION

To investigate the flow and combustion processes in a Solid Fuel Combustion Chamber (SFCC), and to validate its theoretical model, knowledge of temperature and chemical composition, obtained from experiments, is needed. For that reason the main goal of the spectroscopic experiments will be the determination of these quantities as a function of location and time.

This report is limited to a discussion of the spectroscopic method of the determination of the flame temperature in an SFCC.

In chapter 2 some details (only relevant for this investigation) are described briefly about energy levels of diatomic molecules and related spectra. Then the occupation of the energy levels at thermal equilibrium, and problems which arise if the flame is not (enough) transparent, are briefly discussed. As a result of this discussion requirements for the experimental setup are summarized.

Chapter 3 is devoted to a description of the experimental setup.
2: THEORETICAL BACKGROUND

2.1. Energy levels of a diatomic molecule

As a result of previous experiments at the Prins Maurits Laboratory a temperature of ca. 1900 K in a flame of an SFCC was determined [1]. At this gas temperature diatomic molecules (C₂, CO) and radicals like OH will be found. The spectra of these molecules are not complicated with respect to those of polyatomic molecules, while the molecular constants are mostly known [2].

We can distinguish three rather independent (excited) internal energy states, which (normally) in order of decreasing energy are:

1. An electronic state
2. A vibrational state
3. A rotational state.

In the following these states will be discussed separately.

The electronic state is defined by the electron configuration of the molecule. The related energy $E_e$ can only have discrete values.

Classically the molecule can be regarded as an oscillator of two atoms along their connecting line. The energy $E_v$ of the oscillation is quantized and can have one of the values given by [3]:

$$E_v = (v + \frac{1}{2}) \omega \hbar c$$  \hspace{1cm} (1)

where $\omega = 0, 1, 2, \ldots \nu_D$

$\omega$ = a constant, depending on the specific molecule

$\hbar$ = Planck's constant

$c$ = speed of light in vacuum

$\nu_D$ = highest possible value of $v$ of the specific molecule (before dissociation)

This energy $E_v$ is related to the vibrational state $v$.

Classically the molecule can also be regarded as two connected mass centres, rotating about an axis perpendicular to the connecting line and through the common centre of gravity. The related energy $E_r$ of the rotational energy state is given by [3]:

...
\[ E_r = \frac{\hbar^2}{8\pi^2 I} \cdot J(J+1) \]  
\hspace{1cm} \text{(2)}

or

\[ E_r = B J(J+1) \hbar c \]  
\hspace{1cm} \text{(3)}

where \( I \) = moment of inertia of the molecule,

\( B \) = rotational constant of the specific molecule.

Since internal energy exchange is important in the description of the behaviour of molecules, the term (internal) energy levels is used and will be used here.

In Figure 1 a simplified scheme of energy levels of a diatomic molecule has been drawn. A molecule occupies only one of these levels.

2.2. Occupation of energy levels in Boltzmann equilibrium

In the flame of the SFCC the collisional transitions between the energy levels are strongly dominant over the optical transitions. The latter occur by absorption and emission of radiation. In the following we do not take into account the influence of chemical reactions on the level occupation of a part of the molecules studied, the consequences of this influence being beyond the scope of this report.

Under the above conditions the density \( f(E_j) \) of the studied type of molecules, as a function of the internal energy \( E_j \) (obtained by collisions only), is described by the Boltzmann law of internal energy distribution [4]:

\[ f(E_j) = \frac{g_j}{Q} \exp \left( -\frac{E_j}{kT} \right) \]  
\hspace{1cm} \text{(4)}

where \( g_j \) = statistical weight of level \( j \)

\( Q \) = equipartition function

\( T \) = absolute temperature

From eq. (4) we write:

\[ \log f(E_j) = -\frac{1}{kT} E_j + \log g_j - \log Q \]  
\hspace{1cm} \text{(5)}

2.3. Determination of the temperature

For many types of diatomic molecules and diatomic radicals, the values \( g_j \)
Figure 1: Simplified level scheme of a diatomic molecule. For clarity only a few vibrational levels $E_v$ have been depicted, and only two of these have been provided with rotational levels $E_r(J)$. The latter are indicated as smaller horizontal lines.
and $E_j$ in equations (4) and (5) are known. So, to determine $T$, $f(E_j)$ must be measured.

Now, it is important to distinguish three cases:

a) The flame is well transparent for the detected radiation emitted by the molecules studied, and the flame is isothermal,

b) The same as above as far as radiation is concerned, but the flame is not isothermal,

c) The flame is partially absorbing radiation of the detected wavelength region.

Ad a) If the (relative) probabilities for optical transitions from the levels $E_j$ to the ground levels are known from literature and if the relative spectral sensitivity of the complete setup is known (which can be calibrated for), relative values $f_n(E_j)$ of $f(E_j)$ are easily calculated from the measured intensities of the optical transitions from levels $j$. The absolute temperature $T$ of the flame is derived from the slope of the graph where $\log f_n(E_j)$ values have been plotted versus $E_j$ values (see formula 5).

Ad b) Since the slope of the above mentioned graph will be not constant as function of $E_j$, only a mean value of $T$ can be derived. With a flame model, consisting of coaxial shells of different temperature, the measured $f_n(E_j)$-$E_j$ graph is approached by synthesizing $T(r)$ as a function of the radius $r$ of the shell.

Ad c) In this case detectable self absorption occurs. The ratio of line-intensities, integrated over the wavelength, is not representative for the flame temperature as it was in case a. The shell model in ad b now has to be used in an extensive iteration procedure applied to spectra of the flame which have been recorded along lines at various distances from the flame axis.

2.4. Error in temperature measurements

We only discuss the error in $T$ for the simple case a.

From formula (5) we obtain:

$$\frac{\Delta f_n(E_j)}{f_n(E_j)} = \frac{E_j \Delta T}{kT T}$$

(6)
where $\Delta f_n(E_j)$ and $\Delta T$ are the error in $f_n(E_j)$ and, from the latter resulting, error in $T$.

It is clear that

1) the type of molecule should be chosen for maximum height differences in $E_j$, because that choice results in a maximum accuracy of the determination of the slope, discussed in par. 2.3,

2) the relative error in $f_n(E_j)$ should be as small as possible.

The detection frequency will be between 0 Hz and ca. 10 Hz, and can hardly be chosen at will.

Flicker noise is likely to occur in this frequency range. At least the exposure time of each recording should be chosen as to correspond to a frequency which is far below the maximum of the (frequency) spectral flicker noise.

The shot noise should be negligible with respect to the flicker noise.
3. EXPERIMENTAL SETUP

For the experimental setup, the following is required:

1. Regarding the short burning time of the SFCC, the recording of the spectra has to be carried out quickly.

2. Since the SFCC is to be installed in a protective concrete building, the radiation from the SFCC must be conducted along an optical path of about 10 m with sufficient efficiency.

3. The imaging optics in the above mentioned building between the SFCC and the spectroscopic setup should be easily installable and adjustable.

4. The spectral resolution must be large enough to separate the widest rotational lines of diatomic molecules.

Figure 2 is a diagram of the setup.

Radiation from the SFCC is reflected by folding mirror M2 and collimated to a parallel and horizontal beam by lens L1. Between folding mirrors M3 and M4 this beam passes horizontally wall W2 and next traverses the surrounding wall W1 of the concrete building and is brought horizontally to lens L2, which focusses the radiation on the entrance slit S of a grating spectrograph (Jobin Yvon THR 1000S, 2400 groves/mm).

Mirror M1 makes observation of the flame through a window along the axis of the SFCC feasible.

A multichannel plate intensified diode array detector D (SI: IRY 1024, 1024 channels) records ca 100 $\lambda$ of spectra in the visible and UV and resolves ca 0.3 $\lambda$. The recorded spectra are read out by the controller which can store upto 32 spectra. A computer (DEC, Professional 350) processes the obtained spectra.

For wavelength calibration, mirror M5 is inserted, which brings radiation from the wavelength calibration source Li2 (Oriel, pen ray lamp) via lens L4 to S.

To provide easy and quick adjustments of all optical components between S and the SFCC, slit S is illuminated by light from Li 1. This light is brought to an extra exit opening via lens L3 and traverses the spectrograph (set at zero order) in opposite direction to S. From S the beam can easily be followed and adjusted at each optical component.
4. REFERENCES

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Figure 2: Experimental setup.
SFCC : Solid Fuel Combustion Chamber
FL : jet flame
M1,...,5 : folding mirrors
L1,...,4 : imaging lenses
S : entrance slit of the spectrograph
D : intensified diode array detector
W1 : surrounding wall of the concrete building
W2 : wall inside the concrete building
For details, see Chapter 3.