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FTIR analysis of gaseous compounds in the mainstream smoke of regular and light cigarettes

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Abstract

Fourier-transform infrared (FTIR) spectroscopy has been applied to the study of mainstream cigarette smoke from cigarettes of different stated strengths (regular and various light cigarettes with different reported nicotine, tar and CO contents). This technique has allowed for the measurement of a variety of gaseous components including hydrocarbons and both nitrogen and carbon oxides. The results demonstrate that the strength of the cigarette does not have a significant bearing on the quantity of the observed components produced.

Additionally, open-path FTIR studies of diluted sidestream and exhaled smoke have been conducted. These measurements revealed that the majority of gaseous pollutants originated from the sidestream smoke, while the primary smoke was 'purified' or diluted upon exhalation by the smoker.

Keywords: Mainstream cigarette smoke; Light and regular cigarettes; FTIR spectrometry; Gas analysis

1. Introduction

1.1. Methods of analysis of cigarette smoke

Cigarette smoke is a very complex mixture and over the years numerous attempts have been made to identify and quantify its constituents, of which there are tens of thousands. The most common technique used for analysis is gas chromatography (GC). This may utilise, e.g., a nitrogen phosphorous detector (Miyake and Shibamoto, 1995) or be integrated with mass spectrometry (GC–MS) (e.g., Dong et al., 2000; Ding et al., 2005). Proton-transfer-reaction mass spectrometry (Prazeller et al., 1998), time-of-flight mass spectrometry (Dallüge et al., 2002) and capillary electro chromatography (Saeed et al., 1999) have also been applied to study different target analytes in both mainstream and sidestream cigarette smoke. In some cases the whole smoke (i.e. both the solid and the gaseous components) is investigated while in other cases the solid (Ding et al., 2005) and gas phases (e.g., Dong et al., 2000; Cole and Martin, 1996) of the smoke are separated on a Cambridge filter pad. This allows for either or both of the phases to be studied (Parrish et al., 2001). Elsewhere, simultaneous analysis of mainstream and sidestream cigarette smoke has been carried out using quantum cascade laser spectroscopy (Baren et al., 2004; Shi et al., 2003) and also with a tuneable diode laser system, providing millisecond time-resolved measurements (Plunkett et al., 2001).

Fourier transform infrared spectroscopy (FTIR) has, in previous studies, been used to measure gaseous air

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pollutants in the atmosphere (Bacsik et al., 2004, 2005). This method offers the potential for the non-destructive, simultaneous, real-time measurement of multiple gas phase compounds in complex mixtures such as cigarette smoke. Maddox and Mamontov (Maddox and Mamantov, 1977) measured 12 components (in the whole smoke) by means of FTIR using an 18-cm absorption cell. The results were compared puff by puff and from sample to sample. The oxidation of NO to NO_2 and the reaction of these oxides with other smoke components, and the quantitative analysis of these components was studied and the results were compared to model smoke mixtures by Cueto et al. (Cueto et al., 1989; Cueto and Pryor, 1994). Furthermore, on line, real time analysis of mainstream cigarette smoke, with a high precision sampling technique has previously been achieved (Parrish et al., 2001; Li et al., 2002). A special sidestream smoke analysis system has also been built and the results of the measurements compared to the results originating from using standard analytical techniques. Good agreement was found for ammonia and CO_2, but results for CO, HCN and NO differed significantly (Cole and Martin, 1996).

1.2. "Strength of cigarettes"

The strength of a specific cigarette type, e.g., King Size or Ultra Light, is determined by its tar, nicotine and carbon monoxide content. Tar and nicotine yield numbers reported for cigarette brands are not meant to communicate the precise amount of tar or nicotine inhaled by any individual smoker from any particular cigarette. These numbers originate from standardised testing methods, which compare different brands when "smoked" by a machine under identical laboratory conditions. To compare different samples a standard smoking engine is used which allows quantification of the investigated constituents in μg per cigarette (Philip Morris International Management, 2004).

A variety of studies (e.g., Kelbsch et al., 2005; Cummings et al., 2004; Etter et al., 2003) have asked smokers about their reasons for choosing to smoke Light or Ultra Light cigarettes or their reasons for switching to such cigarettes. The results show that the desire to reduce the risk of disease is one of the main factors guiding these choices (National Cancer Institute, 2001). The World Health Organisation however, reports that switching to lower tar products offers no significant health benefits (WHO, 2001). Furthermore, a recent study of six varieties of cigarette (Gendreau and Vitaro, 2005) found that "light" cigarettes do not differ substantially from "regular" cigarettes in terms of smoke yields as determined by a modified ISO method. As a result, smokers of cigarette brands with lower "tar" and nicotine ratings may get as much "tar" and nicotine as smokers of much higher rated brands (Federal Trade Commission, 2000). A recent study (Hecht et al., 2005) showed that there were no statistically significant differences in urinary levels of different lung carcinogens in smokers of regular, light, and ultralight cigarettes.

1.3. Conditions of data acquisition

Most studies comparing the effects of smoking cigarettes of different strengths, e.g., regular and light, focus on measurements of tar and nicotine or some other biomarker (e.g. Benowitz et al., 2005). In this study, it has been investigated as to whether there is a statistical difference in the uptake of gaseous compounds from cigarettes of different advertised "strengths". The method of analysis was FTIR spectrometry employing a simple sampling methodology. This methodology is closer to genuine conditions than that of obtaining results with smoking machines, however while such machines determine yields per cigarette we have evaluated the concentrations of the compounds in a single puff. It has been demonstrated by Maddox et al. (Maddox and Mamantov, 1977), through an investigation of the whole cigarette smoke, that the concentration of the compounds does not change randomly, but instead rises linearly from puff to puff. This means that differences and trends observed in the first puff can be extrapolated to provide information about the entire cigarette. The FTIR technique employed herein is capable only of detecting gas-phase components. As such, any constituents of the smoke present as condensates will not be recorded, however some compounds may be present both as condensates and vapours.

2. Experimental

2.1. Laboratory measurements

Both laboratory (extractive) and field (open-path) spectroscopic measurements have been performed. Laboratory infrared spectra were obtained on a Bio-Rad FTS-185 Series dynamically aligned Fourier transform spectrometer, equipped with a simple 10-cm gas cell of volume 125 ml equipped with an MCT detector.

Measurements were performed by co-adding 64 interferograms. The spectral range was 4000–650 cm^{-1} and the spectral resolution was 0.5 cm^{-1} for all laboratory spectra. "Clean air" spectra were used as the background. These were created by taking a relatively clean air sample to the gas cell from the laboratory.

For quantitative analysis, the region integration and subtraction routine of QASoft software package (Infrared Analysis, 1994) was used and the major absorption band(s) of the selected compounds (Table 1) were accounted for. To aid spectral analysis a library of compound spectra was created. Such a library exists within QASoft for Grams32, however these required to be corrected for slight frequency shifts relative to the samples. The accuracy of the measurements is highly dependent upon the accuracy of the absorption coefficients of the reference spectra. This is estimated to be within ±5% in the QASoft library.