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Caracterización de las emisiones de turbinas
de avión usando espectroscopía FTIR pasiva
con un sistema de visualización

TESIS
Para obtener el grado de
Doctor en Ciencias
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RESUMEN

En la actualidad, la espectroscopía de emisión infrarroja por transformada de Fourier (FTIR, por sus siglas en inglés) se encuentra en una etapa de experimentación y desarrollo con el propósito de ampliar las posibilidades de detección y cuantificación de los principales compuestos de combustión (CO_2 , CO , NO y H_2O) emitidos por turborreactores. Los principales desarrollos tecnológicos en esta área han sido generados como resultado de proyectos financiados por la Comunidad Europea (CE)¹ e investigaciones desarrolladas por el Instituto de Meteorología y Clima del Centro de Investigaciones en Karlsruhe (IMK-IFU, por sus siglas en alemán) con los cuales han sido observadas las principales ventajas operativas de esta técnica sobre la actual metodología de medición reconocida por la Organización Internacional de Aviación Civil (ICAO).

La presente contribución muestra la metodología de medición, el análisis, así como los resultados de la visualización y caracterización de las emisiones de turbinas de avión por espectroscopia FTIR pasiva. Importantes mejoras en la metodología pudieron ser conseguidas a través del innovador sistema de visualización de gases en el infrarrojo (SIGIS, por sus siglas en inglés) y la actualización del código MAPS (Multicomponent Air Pollution Software) para el análisis de los gases. Se presentan en este trabajo los resultados de las investigaciones para el desarrollo de una técnica de validación mediante un quemador diesel y una celda de gas a temperaturas equivalentes a las de los gases de combustión. El arreglo instrumental basado en la espectroscopía pasiva y un sistema de visualización fue probado bajo condiciones reales de operación durante dos campañas de medición en los aeropuertos internacionales de las ciudades de Zurich y de Budapest, al igual que en una cama de pruebas de la compañía desarrolladora de turborreactores Rolls Royce.

¹ AEROJET 1, AEROJET 2, AEROPROFILE, y AEROTEST

ABSTRACT

Fourier Transform Infrared Emission Spectroscopy is a measuring technique in constant development and advances are continuously sought in gas detection and quantification of combustion products (such as CO₂, CO, NO y H₂O) emitted by aircraft engines. The most important contributions in this field are the result of investigations performed by the Institute for Meteorology and Climate Research at the Research Center Karlsruhe (IMK-IFU) and other institutions involved in European Community (CE) ² projects. Those contributions have shown the operative advantages of FTIR spectroscopy over the current measurement methodology currently recognized by the International Civil Aviation Organization (ICAO).

The present contribution shows the measurement methodology, the analysis, the visualization and the characterization of the turbojet emissions performed by FTIR emission spectroscopy. Important improvements in the methodology have been done through the inclusion of a scanning infrared gas imaging system (SIGIS) and the improvement and adaptation of the software MAPS (Multicomponent Air Pollution Software) for the gas analysis. The results of the investigation of a validation technique using a diesel powered burner and a heatable gas cell are also presented in this contribution. The measurement based in passive spectroscopy was tested under real conditions during two measuring campaigns, at Zurich and Budapest International Airports and at a test bed from the company Rolls Royce.

² AEROJET 1, AEROJET 2, AEROPROFILE, y AEROTEST

OBJETIVO

El objetivo general de este trabajo es mejorar el procedimiento de identificación y cuantificación de compuestos emitidos por turborreactores de aeronaves por la técnica FTIR en configuración pasiva. Para este fin se propone hacer uso de herramientas de visualización en el estado del arte para obtener la distribución espacial de las fuentes de emisión a alta temperatura y la inclusión de la función de forma del instrumento (ILS, por sus siglas inglés) en el algoritmo de análisis.

METAS

Se establecieron las siguientes metas específicas con el fin de mejorar la caracterización de emisiones en aeronaves con la técnica FTIR pasiva:

- Reprogramación del algoritmo de análisis cuantitativo MAPS en el lenguaje FORTRAN.
- Adecuación del código fuente para leer y evaluar datos obtenidos con el espectrómetro FTIR marca Bruker, modelo Opag 22.
- Instalación y diagnóstico del sistema de visualización de gases en el infrarrojo (SIGIS) con el espectrómetro Opag 22.
- Elaboración de un método de validación para la medición de gases a altas temperaturas en condiciones controladas: Quemador de flama y celda de gases caliente.
- Realización de campañas de medición en aeropuertos y cama de pruebas para evaluar el desempeño de la metodología.

CAPÍTULO

1

INTRODUCCIÓN

Las turbinas de combustión emiten principalmente dióxido de carbono (CO_2), vapor de agua (H_2O), óxidos de nitrógeno ($\text{NO}_x = \text{NO} + \text{NO}_2$), monóxido de carbono (CO), varios óxidos de azufre (SO_x), hidrocarburos no metanos (NMHC) y partículas, entre otros [Rogers et al., 2005]. Cuando estos compuestos son vertidos en la troposfera alta y estratosfera baja (8 a 12 km), zona conocida como el corredor aéreo, la composición de la estratosfera, principalmente calentada por la absorción de ozono en el ultravioleta, es modificada debido a un desequilibrio en la fuerza radiante (RF) que los productos de combustión, vertidos directamente en ésta, producen en forma de calentamiento o enfriamiento [Sausen et al., 1999].

A nivel regional, los efectos locales en la calidad de aire debidos a la presencia de los aeropuertos son de creciente preocupación, puesto que una gran concentración de contaminantes es emitida sobre áreas relativamente pequeñas. Aunado a esto, en muchas ciudades del mundo las emisiones de automóviles, plantas de energía, refinerías, y otras fuentes importantes están siendo reducidas y sin embargo, las emisiones de los aviones en operaciones aeroportuarias se han incrementado hasta en un 47% entre 1991 y 2000 debido

a la expansión y el éxito de este medio de transporte. La agencia de protección ambiental (EPA) ha estimado que las emisiones de los aeropuertos en 1999 comparadas con las de 1970 son superiores 80% en emisiones de carbón orgánico volátil (VOC) y el doble en óxidos de nitrógeno (NOx) [Unal et al., 2005]. Por tanto, es necesario realizar grandes esfuerzos para mejorar la eficiencia en las aeronaves con el fin de salvaguardar la sustentabilidad ambiental de todo el sistema de transporte aéreo para las futuras generaciones. La intención a futuro y la subsiguiente estrategia del Consorcio Asesor para la investigación Aeronáutica en Europa (ACARE, por sus siglas en inglés), por citar un ejemplo, apuntan sus metas ambientales en la reducción del 50 y 80% de las emisiones pasajero-kilómetro¹ de CO₂ y NO_x, respectivamente para el año 2020 [ver ACARE, 2001].

La Organización Internacional de Aeronáutica Civil (ICAO, por sus siglas en Inglés) dio inicio en 1971 al proceso de regularización de las emisiones de gases producidas por aeronaves. De esta manera, se empezaron a desarrollar los métodos y estándares para la cuantificación y control de las emisiones con el fin de fijar los límites máximos de emisión de hollín, CO₂, CO, NO, H₂O, é hidrocarburos. Todos los turborreactores producidos a partir de esa fecha serían entonces sujetos a esta verificación. Así mismo, se estableció la metodología de muestreo para la cuantificación de estos contaminantes con base en la extracción de muestras y análisis por instrumentos analíticos convencionales y

¹ Unidad de medida de transporte también conocida como (pkm).

que aún es utilizada para estudios de emisiones de motores aéreos [ver ICAO, 1993].

La medición de las emisiones provenientes de motores aéreos es un área de gran relevancia ambiental y con grandes posibilidades de mejorarse ya que la tecnología empleada actualmente es de muy alto costo y técnicamente muy exigente en su operación. La implementación de nuevos métodos que provean una alternativa a los estándares de certificación de la ICAO podría abrir nuevas posibilidades también en el desarrollo de tecnologías de combustión más limpias y eficientes. Por ejemplo, la obtención inmediata de datos de emisión podría ser usada por los fabricantes para optimizar el diseño de las turbinas y los sistemas de control de emisiones. Ha sido demostrado en los últimos años que las técnicas no intrusivas como la espectroscopía FTIR pasiva, tienen un potencial importante para la medición de gases de escape en aeromotores y ya han sido comparadas con métodos *in-situ* (Heland 97 y 98; Schäfer 2000). El éxito de estas investigaciones ha abierto la puerta para nuevos desarrollos que lleven a una metodología capaz de lograr la estandarización.

1.1 Metodología In-situ

El ICAO dio inicio en 1971 a una serie de acciones en el marco de la cuantificación de las emisiones producidas por los motores de las aeronaves entre las cuales se establecieron los estándares iniciales para el control de

emisiones (ICAO, 1993). Dichos estándares, adoptados finalmente en 1981, fijaron los límites máximos de emisión de hollín, CO₂, CO, NO y H₂O e hidrocarburos para los turborreactores producidos a partir de esta fecha. Así mismo, se estableció la metodología de muestreo para la cuantificación de estas especies.

El principio de medición de esta metodología se basa en la extracción de muestras de gas provenientes de diferentes secciones de la pluma de escape. Esto se hace por medio de muestreadores ó líneas de muestreo (ver figura 1.1), que conducen las muestras de gas a instrumentos de medición comercial como; analizadores no-dispersivos por infrarrojo (NDIR), analizadores de ionización de flama (FID, por sus siglas en inglés) y analizadores por quimioluminiscencia.

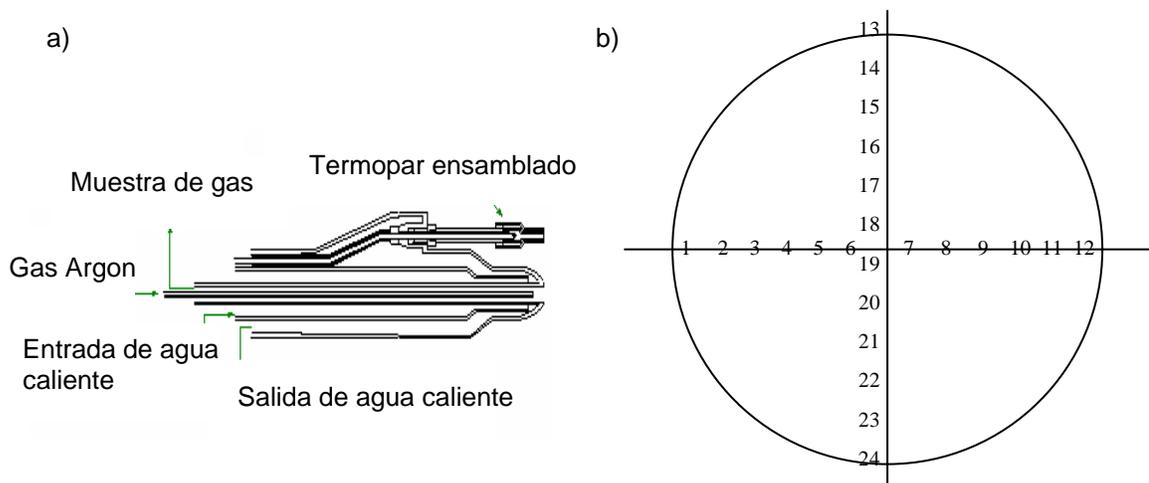


Figura 1.1) a) Esquema del tubo pitot utilizado para la medición de flujo y extracción de gases de escape emitidos por una turbina de gas. b) diagrama de localización de los sitios de extracción en los que es colocado el tubo pitot durante la medición para ser posteriormente transportados hacia los instrumentos de medición in-situ.

Entre las principales desventajas de esta técnica de medición puede mencionarse en primer lugar que cada arreglo instrumental de muestreadores

debe de ser calibrado y específicamente ajustado para cada tipo de motor a ser caracterizado. Por lo mismo, los tiempos de muestreo de cada especie (5 minutos para cada condición de operación del motor) hacen que las campañas de medición por ésta técnica sean extremadamente largas y costosas.

1.2 Metodología No Intrusiva

En la última década se han realizado algunos proyectos de investigación como; AEROJET 1 y 2, AEROPROFILE, AEROTEST, con el fin de proponer nuevos desarrollos tecnológicos en la medición de gases emitidos por los turborreactores de las aeronaves. En ellos se mostró que la técnica de percepción remota por espectroscopía FTIR ofrece importantes ventajas sobre la metodología planteada por ICAO como: bajo costo de operación, fácil manejo de la medición, posibilidad de mediciones en tiempo real, menor tiempo de muestreo (debido a la medición simultánea de especies) y posibilidad de realizar mediciones de un motor antes de su instalación en una aeronave así como durante condiciones normales de operación.

El principio de medición de esta técnica se ilustra en la figura 1.2. La radiación infrarroja emitida por los gases calientes de combustión viaja a través de la atmósfera hasta llegar al espectrómetro. Un telescopio concentra la radiación originada de un punto o área reducida de la pluma y es dirigido manualmente hacia las posiciones donde la intensidad máxima de la radiación infrarroja es detectada. Esto se hace con el fin de obtener la mejor relación señal ruido en los

espectros. Una vez obtenidos los espectros, la interpretación de éstos es realizada por programas de cálculo basados en modelos de transferencia de radiación y ajustes con espectros de referencia mediante regresiones numéricas.

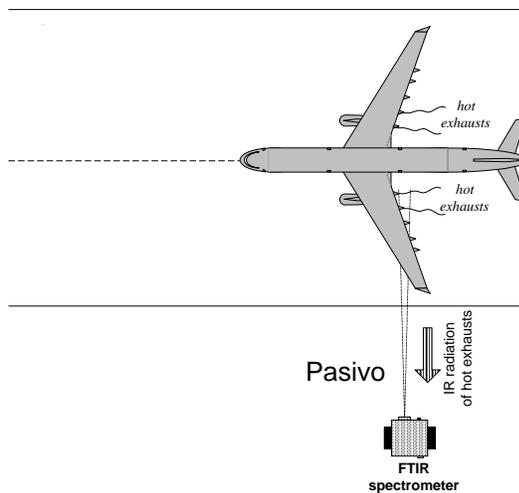


Figura 1.2 Configuración de las mediciones realizadas por el IFU con técnicas percepción remota (configuración pasiva y activa) para determinar emisiones de CO y NO producidas por aeronaves².

El IMK-IFU (Institut für Meteorologie und Klima Forschung – Institut für Atmosphärische Umweltforschung) en Alemania, ha realizado mediciones con esta configuración utilizando un espectrómetro Kayser-Threde GmbH modelo K300, a una resolución de 0.2 cm^{-1} [Kayser-Threde, 1992]. Para el análisis de los espectros, este grupo desarrolló el software MAPS (Multicomponent Air Pollution Software), el cual produce espectros sintéticos a través del uso de un método línea-por-línea (LBL, por sus siglas en inglés) y que los ajusta al espectro medido mediante una regresión por mínimos cuadrados. La incertidumbre reportada para los cálculos de estas mediciones es de $\sim 30\%$, teniendo como contribución principal la base de datos espectrales HITEMP ($\sim 15\%$) y en la conversión de los datos moleculares a alta temperatura (detalles en Heland et al., 1997 y 1998).

Las mediciones realizadas revelaron que el éxito de las mediciones dependía ampliamente en la habilidad del operador del instrumento para dirigir el telescopio a una posición óptima dentro de la pluma de gases de emisión. Por otro lado, debido a que las aeronaves en ocasiones se encontraban a distancias mayores a los 50 m y era escaso el tiempo mientras éstas no estaban en movimiento, la obtención de espectros de emisión útiles para el análisis era un reto.

Para este trabajo de investigación, y con el objetivo de mejorar la técnica de medición, se planteó la siguiente hipótesis:

Es posible mejorar significativamente la técnica de detección remota por FTIR pasivo implementando un sistema de visualización capaz de proporcionar con rapidez la distribución espacial de los contaminantes en la pluma de escape antes de obtener la medición del espectro de emisión para su caracterización.

Para lograr este fin, se elaboró un convenio de colaboración entre el IMK-IFU y la Universidad Tecnológica de Hamburgo Harburg (TUHH) para el desarrollo de un sistema de visualización automática de plumas de gas a alta temperatura. Esta colaboración tuvo como resultado la adaptación de un dispositivo que la TUHH ya venía desarrollando específicamente para el espectrómetro FTIR Bruker, modelo Opag22, pero con diferentes aplicaciones.

2

METODOLOGÍA

2.1 Introducción a la espectroscopia FTIR pasiva

La espectroscopia infrarroja trabaja, gracias a que las moléculas poliatómicas o moléculas diatómicas heteronucleares relevantes para la atmósfera como H₂O, CO₂, O₃, N₂O, CO, CH₄, NO, SO₂, NO₂, NH₃, HCl, HCHO, C₂H₆, y otras, cuentan con transiciones rovibracionales (rotación y vibración) activas en esta región del espectro electromagnético. Las energías de estas transiciones y los parámetros moleculares en el infrarrojo fundamental ó el infrarrojo medio, que abarca la región de 700 a 3500 cm⁻¹ (2.9 -14.3 μm), son bien conocidos y pueden ser consultados en la literatura o en bases de datos que son periódicamente actualizadas como HITRAN, ATMOS ó GEISA [Rotman et al., 1992, Brown et al., 1987 Husson., 1994]. Dichos parámetros pueden ser utilizados para calcular espectros de transmisión o absorción a lo largo de una capa de gas homogénea a temperaturas y presiones conocidas. En el caso de un paso óptico no-homogéneo, éste puede ser dividido en subcapas homogéneas de las cuales su transmisión puede ser obtenida y la transferencia de radiación a través del medio puede entonces ser calculada. En la siguiente sección se desarrolla, en forma detallada, del principio físico-matemático del modelo de transferencia de

radiación utilizado en esta contribución. Así mismo, se profundiza de manera clara en los conceptos esenciales de la espectroscopía de emisión para su claro entendimiento.

2.1.1 Ecuación de transferencia de radiación.

Por definición, si un haz de radiación infrarrojo es conducido a través de un espacio en el cual no existen moléculas activas en el infrarrojo (descartando otros procesos de extinción), la radiación final obtenida será igual a la radiación inicial emitida. En el caso de que a lo largo de ese paso óptico (s) haya un gas activo absorbiendo en la misma frecuencia del haz, la radiación inicial (I_0) sufrirá una disminución en su intensidad (I) tal como lo describe la ley de Beer Lambert-Bouguer

$$\frac{dI}{ds} = -k\rho_a I \quad , \quad (2.1)$$

en donde k es el coeficiente de absorción (en unidades de m^2/kg), ρ_a es la densidad del absorbedor (kg/m^3) é I es la intensidad de radiación que depende de la longitud de onda. Nótese que la intensidad es dependiente de si misma, y proporcional a la densidad de materia absorbente. Si asumimos que k y ρ_a son constantes, podemos resolver la ecuación (2.1)

$$I(s) = I(s=0)e^{-k\rho_a s} \quad , \quad (2.2)$$

sustituyendo

$$\tau = k\rho_a s \quad (2.3)$$

en (2.2), esta se puede transformar en

$$I(\tau) = I(\tau = 0)e^{-\tau}, \quad (2.4)$$

En donde $I(\tau)$ desde el punto de vista óptico, es una medida del espesor óptico lo cual puede traducirse en que la intensidad I decrece proporcionalmente a $1/e$.

Si el gas expuesto a la radiación también emite radiación, que es justamente el caso de estudio en este trabajo al tratarse de compuestos de gas caliente, entonces la ecuación (2.1), se convierte en

$$\frac{dI}{ds} = -k\rho_a I + k\rho_a B, \quad (2.5)$$

en donde $k\rho_a B$ será la radiación térmica emitida por el gas absorbedor.

En este modelo simplificado, no están considerados:

- La dispersión, sólo absorción y emisión.
- Si $I = B$, entonces la intensidad restante I permanecerá constante. En otras palabras, la absorción debida por el medio esta balanceada por la radiación emitida por el medio.
- La constante de absorción k es una función de ν (la frecuencia), como lo es B . Por lo que I es generalmente una función de frecuencia.
- El caso especial de k independiente de la frecuencia es llamado el caso gris.

- $B=0$ es una buena aproximación para radiación solar en la atmósfera sin considerar dispersión y la absorción de especies como el carbón negro.

La ecuación de transferencia de radiación (2.5), es una combinación de la ecuación de extinción, (2.1), y la función de la fuente, compuesta por $+K\rho_a B$ en donde $k\rho_a$ será sustituida por β , definida como el coeficiente de volumen de extinción. Para esta nueva ecuación, el paso óptico esta dividido en capas homogéneas y discretas en las cuales se asume el equilibrio termodinámico.

$$\frac{dl_\sigma}{ds} = -\beta l_\sigma + \beta B_\sigma \quad (2.6)$$

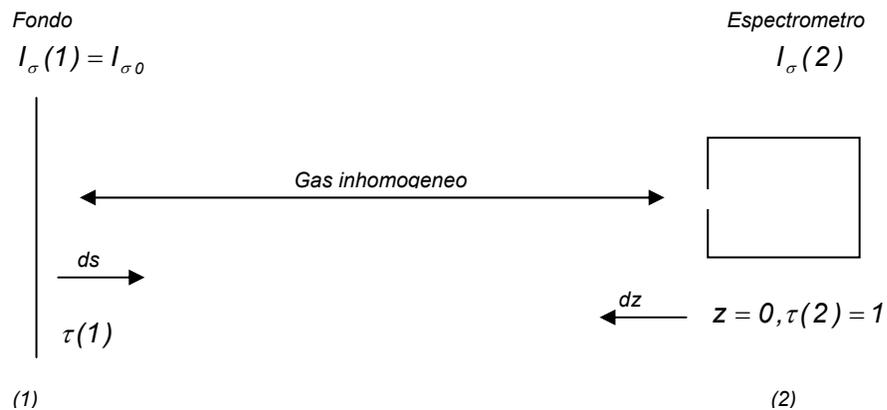


Figura 2.1. Esquema de transporte de radiación [Heland et al, 1997].

2.1.2 Solución de la ecuación de transferencia de radiación.

Introduciendo la ecuación de transmisión,

$$\tau = e^{-u(z)}, \quad (2.7)$$

en la cual u representa al paso óptico expresado como:

$$u = -\int_{z=0}^z \beta(z) dz \quad (2.8)$$

y debido a que la dirección de la propagación de la radiación (Figura 2.1) es negativa, asumimos a du como:

$$du = \beta(z) = -\beta(s). \quad (2.9)$$

Derivando la ecuación de transmisión

$$d\tau = -\beta ds \exp^{-u(z)}, \quad (2.10)$$

obtenemos

$$ds = -\frac{1}{\beta\tau} d\tau. \quad (2.11)$$

Para simplificar, introducimos la ecuación (2.11) en

$$dl_\sigma = \beta(-l_\sigma + B_\sigma) ds, \quad (2.12)$$

y de esta manera podemos obtener que

$$\tau dl_\sigma + l_\sigma d\tau = d(l_\sigma \tau) = B_\sigma d\tau. \quad (2.13)$$

Esta ecuación puede ser integrada de la siguiente forma

$$\tau(2)l_\sigma(2) - l_\sigma(1)\tau(1) = \int_{\tau(1)}^{\tau(2)} B_\sigma d\tau. \quad (2.14)$$

Considerando las condiciones de frontera en las que $\tau(2) = e^{-u(0)} = 1$ en la posición 2 (Figura 3.1) y $I_\sigma(1) = I_{\sigma,0}$, la ecuación final puede ser escrita de la siguiente forma:

$$I_\sigma(2) = I_{\sigma,0}\tau(1) + \int_{\tau(1)}^1 B_\sigma d\tau \quad (2.15)$$

en donde tenemos la suma de una porción $I_{\sigma,0}(1)\tau(1)$, que es la caracterización de la absorción del fondo, y una integral en la cual la radiación de la mezcla depende de su temperatura. Considerando una capa homogénea, en donde se considera cada capa de espesor l a temperatura, presión y concentración constante.

$$B_\sigma(T_n) = B_{\sigma,n}; U_n = \beta_n l_n; \tau_{gas} = \prod_{n=1}^k \tau_n \quad (2.16)$$

Nuestra ecuación quedará de la siguiente forma

$$I_\sigma(2) = I_{\sigma,0}\tau + (1-\tau)B_\sigma \quad (2.17)$$

y para un sistema de multicapas, ésta puede escribirse como:

$$I_\sigma = \tau_m I_{\sigma,m-1} + (1-\tau_m)B_\sigma(T_m). \quad (2.18)$$

2.2 Análisis mediante el software MAPS

2.2.1 Descripción

En forma resumida, el software de análisis Multicomponent Air Pollution Software (MAPS), descrito anteriormente por Haus, et al. (1991) y Heland et al. (1997), se utiliza para calcular una serie de espectros de emisión en el infrarrojo, llamados espectros de referencia o espectros de calibración. Éstos son aproximados al espectro medido del cual se pretende extraer información acerca de su concentración y temperatura. Los espectros de calibración son generados en un principio a partir de un modelo de transferencia de radiación en el cual el paso óptico es dividido en subcapas homogéneas a temperatura y presión constantes. Dentro de la estructura del modelo de transferencia de radiación se encuentra un submódulo para la determinación de los estados apropiados de absorción/emisión que incluye un algoritmo matemático para la conversión de parámetros espectroscópicos individuales como son la magnitud de las transiciones gobernadas por los estados basales de población, la probabilidad de que una transición ocurra entre estados altos y bajos, así como el estadísticamente apropiado factor de forma. Estos parámetros son tomados de la base de datos HITRAN y HITEMP [Rothman et al., 1995 y 1997]. Finalmente para completar el cálculo de los espectros sintéticos, MAPS convolucionada al espectro medido con la forma de línea, función que incluye todos los parámetros del instrumento. Una vez finalizada la creación de los espectros sintéticos, el o

los espectros desconocidos son ajustados al espectro medido mediante el método clásico por mínimos cuadrados (CLS, por sus siglas en inglés).

2.2.2 Simulación de espectros sintéticos basado en cálculos LBL.

El modelo línea-por-línea (LBL, por sus siglas en inglés) tiene el objetivo de realizar la conversión de parámetros espectroscópicos individuales como: la magnitud de las transiciones gobernadas por los estados basales de población, la probabilidad de que una transición ocurra entre estados altos y bajos y el estadísticamente apropiado factor de forma, a espectros con condiciones de temperatura deseadas tomando en cuenta la transmitancia y absorbancia del medio.

Con este propósito es necesario describir el coeficiente de absorción en función de la frecuencia. Debido a que en nuestro modelo cada uno de los compuestos contribuye a la señal detectada en la corriente de gas, es imprescindible considerar el volumen de coeficiente de absorción $\beta(\sigma)$ como:

$$\beta = \sum_{\text{gases}} n_i \cdot k_i, \quad (2.19)$$

en donde k_i es el coeficiente de absorción espectral de la molécula a temperatura y presión dadas (incluyéndose la suma de todas las contribuciones i) y n_i es la densidad en número.

El coeficiente de absorción, el cual puede ser expresado de forma similar como la contribución de todas las líneas individuales j (transiciones) de un número de especies químicas i , es descrito en la siguiente ecuación

$$ki(\sigma, T, p) = \sum_j S_{ij}(T) f_{ij}(\sigma - \sigma_j^0 | \sigma_j^0, T, p), \quad (2.20)$$

en donde S_{ij} ($\text{cm}^{-1}/\text{molécula cm}^{-2}$) es la fuerza o intensidad de línea y f_{ij} el factor de forma que describe el mecanismo físico del ensanchamiento de las líneas.

La intensidad de línea, S_{ij} , es dependiente de la temperatura a través del factor de Boltzmann y la función de partición, que es dada por el producto de las funciones de partición independientes asociadas a los modos vibrarotacionales y electrónicos:

$$S_{ij}(T) = S_{ij}(T_0) \cdot \frac{e^{-\frac{E_j}{K_B T}}}{e^{-\frac{E_j}{K_B T_0}}} \cdot \frac{1 - e^{-kT}}{1 - e^{-kT_0}} \cdot \frac{Q_{rot}(T_0)}{Q_{rot}(T)} \cdot \frac{Q_{vib}(T_0)}{Q_{vib}(T)} \quad (2.21)$$

en donde $S_{ij}(T_0)$ es el valor de intensidad de la línea a temperatura estándar (296K) y σ_j^0 es el valor de línea central en cm^{-1} (ambos obtenidos del banco de parámetros moleculares HITRAN a 296K y 1013.25 mbar) que finalmente son

convertidos a la temperatura deseada (T). Q_{rot} y Q_{vib} son las funciones particionales de rotación y vibración, E_1 es la energía del estado más bajo de la transición (cm^{-1}) y k_B es la constante de Boltzmann (1.3806×10^{-23} J/K).

La dependencia de temperatura de la función de partición rotacional Q_{rot} es calculada con la siguiente ecuación:

$$\frac{Q_{rot}(T_0)}{Q_{rot}(T)} = \left(\frac{T_0}{T}\right)^r \quad (2.22)$$

En la ecuación 2.22, el exponente r es el valor de la amplitud de la molécula (por ejemplo: CO=1, H₂O=0.5, SO₂=1.5). Las funciones particionales de vibración pueden ser calculadas de igual forma a partir de:

$$Q_{vib} = \prod_{k=1}^n \left[1 - e^{-\frac{hc\sigma_k}{KT}} \right]^{-d_k}, \quad (2.23)$$

en donde h es la constante de Planck (6.6626×10^{-34} J seg), C la velocidad de la luz (2.9979×10^8 m/s), σ_k el número de onda y d_k es el grado isoenergético del respectivo modo oscilatorio (Heland, 1996).

2.2.3 Factor de forma

Cuando la luz que ha sido absorbida o emitida por una molécula se examina espectralmente a detalle, se puede observar que ésta se encuentra absorbida o emitida sobre un ancho de banda finita debido al efecto llamado ensanchamiento de banda.

Este ensanchamiento es debido al movimiento de translación de las moléculas, y a la distorsión inducida producida por la presencia de otras. El ensanchamiento de banda debido al efecto Doppler, producto de la distribución estadística de los desplazamientos en ambas direcciones, es dependiente de la temperatura. Este es un factor dominante en el ensanchamiento de banda de moléculas presentes a alturas superiores a los 40 km. Por otro lado, el ensanchamiento provocado por la presencia de otras moléculas es llamado el efecto Lorentz y este efecto es dependiente tanto de la presión como de la temperatura. El efecto Lorentz domina los efectos de ensanchamiento debajo de los 10 km de altura.

La función de ensanchamiento Doppler puede ser descrita por la siguiente ecuación

$$\alpha_D = \frac{\sigma_j^0}{c} \cdot \sqrt{\frac{2k_B T}{m} \ln(2)} = 3.586 \cdot 10^{-7} \sigma_j^0 \cdot \sqrt{\frac{T}{M}}, \quad (2.24)$$

mientras que la función de ensanchamiento por el efecto Lorentz es descrita por

$$\alpha_L = \alpha_{L0}(p_0, T_0) \cdot \left(\frac{P}{P_0} \right) \cdot \left(\frac{T_0}{T} \right)^\gamma, \quad (2.25)$$

en donde m es la masa molecular, c la velocidad de la luz, M la masa molar, y γ el exponente de temperatura. En nuestra aplicación, debido al análisis de una mezcla de gases calientes, el efecto de ensanchamiento Doppler y Lorentz (α_D y α_L) es del mismo orden, por lo que ambas son convolucionadas obteniéndose así una función de perfil Voigt, descrita por la integral (2.26) [Haus et al., 1991].

$$f_M(\sigma, p, T) = \frac{a}{\pi\sqrt{\pi}} \frac{2\sqrt{\ln 2}}{\alpha_D} \int_{-\infty}^{+\infty} \frac{e^{-y^2}}{(x-y)^2 + a^2} dy, \quad (2.26)$$

en donde

$$x = \frac{\sigma - \sigma_0}{\alpha_D} \sqrt{\ln(2)} y = \frac{\sigma' - \sigma_0}{\alpha_D} \sqrt{\ln(2)}, \quad (2.27)$$

$$a = \frac{\sigma_L}{\alpha_D} \sqrt{\ln(2)}. \quad (2.28)$$

Lamentablemente, esta integral no puede ser resuelta por métodos analíticos pero sí por aproximaciones que describen el perfil Voigt y una expresión racional que describe el ancho de la forma de la línea. Matvejev, et al. (1972) propuso que el factor de forma de $f_M(\sigma, p, T)$ pudiera ser escrito como

$$f_M(\sigma, p, T) = \frac{1}{\pi\alpha_V} (f_1 + f_2 - f_3) \quad (2.29)$$

en donde

$$\alpha_V = \frac{1}{2}\chi + \frac{1}{20}\alpha_L \left(1 - \frac{2\alpha_L}{\chi}\right), \quad (2.30)$$

$$\chi = \alpha_L + \sqrt{\alpha_L^2 + \alpha_D^2}, \quad (2.31)$$

$$f_1 = \sqrt{\pi} \cdot (1 - \xi) e^{-\eta^2 b^2}, \quad (2.32)$$

$$f_2 = \frac{\xi}{1 - \eta^2} \quad (2.33)$$

y

$$f_3 = \left[\xi \cdot (1 - \xi) \cdot \left(\frac{1.5}{b^2} + 1 + \xi \right) \right] \cdot \left[0.066 e^{-0.4\eta^2} - \frac{1}{40 - 5.5\eta^2 + \eta^4} \right] \quad (2.34)$$

considerando

$$\eta = \frac{\sigma - \sigma_j^0}{\alpha_V}, \xi = \frac{\alpha_L}{\alpha_V}, b = \sqrt{\ln(2)}. \quad (2.35)$$

El parámetro η caracteriza la sobreposición de líneas, así como la consideración de la contribución de todos los centros de línea en la integración sobre el número de onda. La sobreposición de estas líneas es básica, por lo cual el coeficiente de absorción K_Δ integrado sobre el número de onda en el

procedimiento numérico LBL se basa esencialmente en considerar sólo líneas y no en cuantificar intervalos $\Delta\nu$.

2.2.4 Calibración radiométrica del espectro

Debido a que los espectros de emisión sintéticos son calculados en unidades de radiancia (Watts sobre estereorradián por centímetro cuadrado por centímetro) y el espectro medido (crudo) está en unidades de intensidad relativa, éste tiene que ser transformado a la misma unidad que los espectros sintéticos a través de un cálculo que comprende la medición de radiación emitida por un cuerpo negro (objeto que absorbe o emite toda la luz y toda la energía que incide sobre él) a temperatura y emisividad (ϵ) conocidas.

Debido a que la intensidad del instrumento M_σ es una combinación de la intensidad de la fuente I_σ y la radiación propia G_σ del instrumento, ésta se puede escribir como

$$M_\sigma(\sigma, T_{source}, T_{instr}) = E(\sigma, T_{instr}) \times [G_\sigma(\sigma, T_{instr}) + I_\sigma(\sigma, T_{source})], \quad (2.36)$$

en donde la sensibilidad espectral E contiene la conversión de unidades.

Utilizando a dos espectros de referencia del cuerpo negro a diferentes temperaturas $M_{\sigma,1}$ y $M_{\sigma,2}$ con intensidades conocidas $I_{\sigma,i} = \varepsilon X B_{\sigma,i}$, se obtienen

$$E = \frac{1}{\varepsilon} \left(\frac{M_{\sigma,1} - M_{\sigma,2}}{B_{\sigma,1} - B_{\sigma,2}} \right) \quad \text{y} \quad (2.37)$$

$$G_{\sigma} = \frac{\varepsilon}{2} [(x-1)B_{\sigma,1} - (x+1)B_{\sigma,2}] \quad (2.38)$$

en donde $x = (M_{\sigma,1} + M_{\sigma,2}) / (M_{\sigma,1} - M_{\sigma,2})$. Cada punto del espectro individual medido $M_{\sigma}(\sigma_n)$ en un rango de longitud de onda de $\Delta\sigma \approx 10 \text{cm}^{-1}$ tiene que ser convertido entonces a unidades de radiancia $I_{\sigma}(\sigma_n)$ con el valor medio de G_{σ} y E en $\Delta\sigma$:

$$I_{\sigma}(\sigma_n) = \left[M_{\sigma}(\sigma_n) / \bar{E} \right] - \bar{G}_{\sigma}. \quad (2.39)$$

Heland et al. (1997) encontró que para el caso de un espectrómetro común, la radiación propia del instrumento en el infrarrojo intermedio es equivalente a una temperatura de cuerpo negro de $\sim 10^{\circ}\text{C}$. Por lo tanto, al comparar el resultado de intensidad con respecto a 200°C del cuerpo negro, la radiación propia en la ecuación (3.31) del instrumento equivale aproximadamente al 2%, por lo cual puede ser despreciado para nuestro propósito. De esta manera, la ecuación 2.40 es utilizada para efectuar la calibración de los espectros de emisión

$$I_{\sigma}(\sigma, T_{source}) = \varepsilon B_{\sigma}(\sigma, T_{ref}) \left[\frac{M_{\sigma}(\sigma, T_{fuente})}{M_{\sigma}(\sigma, T_{ref})} \right] - G_{\sigma}(\sigma, T_{instrumento}). \quad (2.40)$$

2.2.5 Simulación de cada punto individual de medición.

Teóricamente, el coeficiente de absorción (ecuación 2.20) en un intervalo espectral debe ser continuamente calculado y las contribuciones de todas las líneas espectrales de la molécula, en el número de onda σ , deben de ser tomadas en cuenta. Desafortunadamente, esto requeriría una cantidad enorme de operaciones que tendrían que ser calculadas por lo que MAPS pretende realizar una simulación satisfactoria sólo con algunos puntos medidos por el interferómetro.

Para simular un punto medido en $\Delta\sigma$, es indispensable contar con suficientes valores de intensidad teórica (I_{σ}^{th}) dentro de la resolución espectral para así incluir la función de forma del instrumento (ILS).

$$I_{\sigma}^{I,A}(\sigma_{Mess}) = (I_{\sigma}^{th} * ILS)_{en\delta\sigma en\sigma_{Med}}, \quad (2.41)$$

La ILS es una función que caracteriza la influencia del espectrómetro sobre el espectro medido y es también vista como la forma de un espectro de radiación monocromática calculado por la Transformada de Fourier.

Hase et al. (1999) han observado que en el área de espectroscopia a alta resolución, esta función es casi por lo general considerada como simétrica y perfecta y no siempre es así, teniéndose como riesgo principal de esta consideración la introducción de un error sistemático al análisis cuantitativo de las especies de interés. Por tal razón, la caracterización de la ILS se vuelve prioritaria en este trabajo.

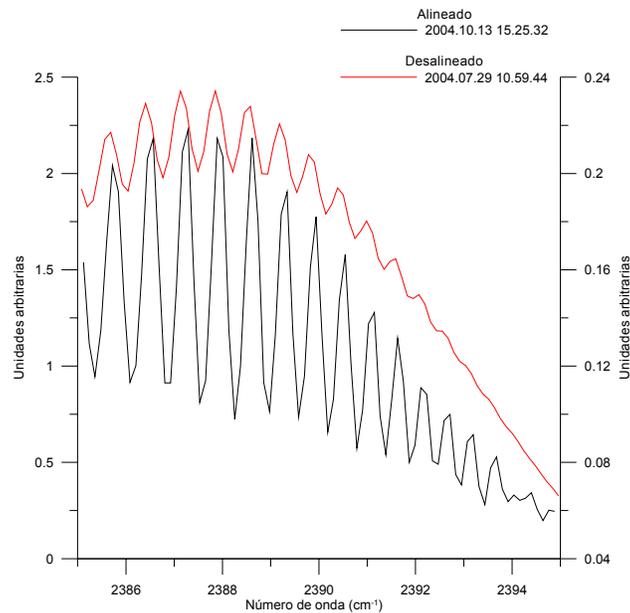


Figura 2.2. Espectros de emisión a alta resolución capturados por el Opag 22 en dos fechas distintas: antes y después de una realineación de la óptica interna llevada a cabo por el fabricante. En la figura correspondiente al espectro medido con el espectrómetro desalineado puede observarse un error de fase y un ensanchamiento de banda considerables (sección 2.2.3).

Existen varias maneras de caracterizar y ajustar la función ILS de un espectrómetro FTIR para que los espectros sintéticos ideales se ajusten a la influencia real del espectrómetro. Por citar algunos ejemplos, Hase et al. (1999) han caracterizado la función ILS de espectrómetros a alta resolución (0.001 cm^{-1}) a través de mediciones en celda de gas y simulaciones realizadas con el software LINEFIT. Por su parte, Haro et al. (2000) han propuesto un método matemático para la detección y corrección al igual que Allout et al. (1998), el cual propone una expresión analítica generalizada para esta función la cual, según los autores, tiene la posibilidad de eliminar errores en los parámetros de línea inducidos por asimetría en perfiles de línea y errores de fase debidos a una posible variación de la energía recibida por el detector durante el registro de los interferogramas. Otros autores como Griffith et al. (1996) y Esler et al. (2000), han propuesto una solución integral incluida en el software Multiple Atmospheric Layer Transmisión (MALT) a través del cual espectros sintéticos con ILS ajustables son generados con 3% de incertidumbre, según los autores.

En esta contribución, la función ILS del espectrómetro Opag 22, fue caracterizada utilizando una celda de gas y el módulo de cálculo GeDetekt-ILS propuesto por Harig et al. (2004). En la siguiente sección se presenta el principio teórico y el modelo experimental para la determinación de la función ILS.

2.3 Determinación de la función de forma del instrumento

2.3.1 Base teórica

Harig, (2004) estableció que el espectro $S^c(\sigma)$ calculado por la transformada de Fourier del interferograma puede ser escrito como

$$S^c(\sigma) = \int_{-\infty}^{\infty} S(\sigma') A(\sigma - \sigma', \sigma') d\sigma', \quad (2.42)$$

en donde $S(\sigma)$ es el espectro real medido con una diferencia de paso óptico infinita y radiación colimada. $A(\sigma, \sigma')$ es la función ILS a la frecuencia σ' , que puede entenderse como la forma del espectro calculado de radiación monocromática a una frecuencia σ' . Para un interferómetro ideal, libre de aberraciones ópticas que opere con radiación perfectamente colimada, la función ILS A_0 , es dada por la transformada de Fourier de la función que describe el movimiento finito del espejo ó por la función de apodización que es por definición una función ideal.

La función de apodización describe la truncación de señal como el producto de la señal original y la función de truncación, que es usualmente llamada función furgón (Boxcar, en idioma inglés. Ver figura 2.3) descrita como:

$$\Pi\left(\frac{x}{2D}\right) = \begin{cases} 0, & \\ 1/2, & \left| \frac{x}{2D} \right| = \begin{cases} > 1/2 \\ = 1/2 \\ < 1/2 \end{cases} \\ 1, & \end{cases} \quad (2.43)$$

Aplicándole a la ecuación 2.43 la transformada de Fourier en unidades de amplitud que se extienden desde $+D$ a $-D$ obtendremos la función ILS (figura 2.3) de un interferómetro ideal y libre de aberraciones ópticas que opera con radiación perfectamente colimada.

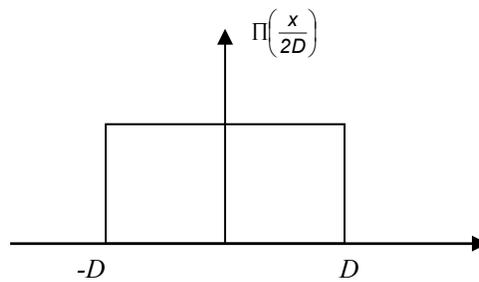


Figura 2.3. La función de truncación de señal de caja.

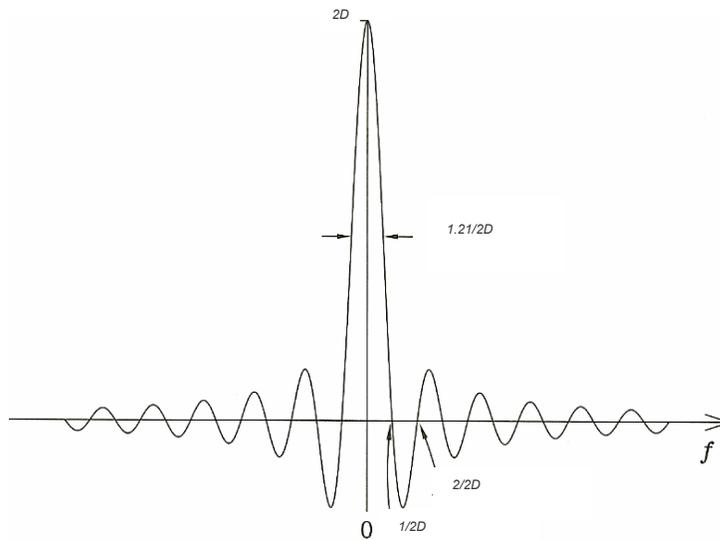


Figura. 2.4. Transformada de Fourier de la función furgón de unidad de amplitud que se extiende desde $+D$ a $-D$.

El efecto de multiplicar el interferograma $S^c(\sigma')$ por la función (2.43) puede visualizarse de la misma manera como la convolución de la transformada de

Fourier del interferograma medido con la transformada de Fourier de la función (2.43) que resulta en la función (2.45).

$$A(\sigma, \sigma') = A_0(\sigma) = 2D \operatorname{sinc}(2\pi D\sigma), \quad (2.45)$$

Aquí D es el paso óptico máximo en el interferómetro. En esta función, la ILS es independiente de σ' y la integral en la ecuación (2.42) se convierte en una integral de convolución. En la práctica, en especial en el caso de un interferómetro optimizado para alto rendimiento, rayos no paraxiales de la fuente finita, que subtienden un ángulo sólido Ω en el interferómetro, se enfocan al detector (debido a el área finita del detector) causando un ensanchamiento de la ILS y un desfase en la frecuencia, por lo que la ILS será dada por la convolución de:

$$A(\sigma, \sigma') = A_0(\sigma) * A_{inh}(\sigma, \sigma'). \quad (2.46)$$

en donde $A(\sigma, \sigma')$ es la función que describe el efecto de ensanchamiento y el desfase de frecuencia.

En el caso de una fuente homogénea y un interferómetro de Michelson (con espejos ideales), en los cuales la radiación que sale del interferómetro es medida por un detector en el plano focal de un lente condensador (o espejo), $A_{inh}(\sigma, \sigma')$ es una función rectangular (de furgón) de un ancho total $\sigma'\Omega/2\pi$, centrada en $\sigma' = \sigma'\Omega/4\pi$. La función (2.46) incluye en si misma efectos como el de una

fuente de radiación fuera de foco, un interferómetro sin colimador ni condensador y el efecto de desalineación del interferómetro.

Finalmente, un espectro calculado puede ser aproximado a un espectro medido por la convolución del espectro sintético con la función del instrumento en σ' dentro de una pequeña región espectral $\Delta\sigma_{SR}$ menor a σ'

$$S^c(\sigma) = S(\sigma) * A(\sigma, \sigma'). \quad (2.47)$$

La función del instrumento citada es válida en casos especiales. Ésta describe el efecto de una desalineación ó una fuente fuera de foco del interferómetro. En orden de caracterizar la combinación de los efectos de aberración, desalineación, movimientos no lineales de los espejos, etc, puede ser utilizada una función instrumental empírica.

Para nuestra investigación son utilizadas dos ILS. Para el cálculo teórico es empleada una ILS ideal (A_0). Para modelar el espectro medido, es calculada una ILS usando una función del instrumento inherente definida por cinco parámetros $p_1 \dots p_5$:

$$A_{inh}(\sigma, \sigma') = \begin{cases} 0 & \text{for } \sigma < -p_1 \\ p_2 + p_3(\sigma + p_1)^2 & \text{for } -p_1 \leq \sigma \leq -p_4 \\ p_5 \text{rect} \left(\frac{\sigma + \frac{p_4}{2}}{p_4} \right) & \text{for } \sigma > -p_4 \end{cases} \quad (2.48)$$

Este modelo (ecuación 2.48) contiene la función inherente de un interferómetro de Michelson ideal, iluminado por una fuente homogénea extendida y es una aproximación a la función inherente del interferómetro sin colimador ni condensador¹⁴.

2.3.2 Procedimiento experimental

Con el objetivo de caracterizar la función ILS de nuestro espectrómetro, se midieron espectros de absorción (L_{med}) de una especie de gas conocida y se crearon una serie de espectros de calibración (L_{model}) a diferentes concentraciones utilizando como principio la siguiente función

$$\sum_{i=1}^N (L_{model}^i - L_{med}^i)^2 = \min, \quad (2.49)$$

en la cual N es el número de elementos del espectro. Para llevar a cabo esta labor, se utilizó un módulo especial del software GeDetekt llamado "ILS module" el cual incluye a dos sub-módulos de cálculo. El primero, basado en el principio físico visto en la sección anterior 2.3.1, es un módulo para la determinación de la función ILS y el segundo es un modelo de transferencia de radiación de tres capas (ecuación 2.30)

$$L_S = (1 - \tau_{at})B_{at} + \tau_{at} [(1 - \tau_c)B_c + \tau_c L_b], \quad (2.50)$$

en donde τ_{at} es la transmitancia de la atmósfera entre el espectrómetro y la nube, B_{at} es la radiación espectral del cuerpo negro a la temperatura de la atmósfera, τ_c es la transmitancia de la nube, y B_c es la radiación espectral de un cuerpo negro a la temperatura de la nube T_c . L_b es la radiación que entra en la capa de la nube proveniente del fondo. El coeficiente de dispersión en la región espectral infrarroja es bajo por lo que la contribución de este efecto es despreciada.

Si consideramos la temperatura de la nube y las capas atmosféricas como iguales, la ecuación (2.50) queda como

$$L_s = B_{at} + \tau_{at}\tau_c(L_b - B_{at}) \quad (2.51)$$

y la diferencia de radiación es $\Delta L = L_s - L_b$ dada por:

$$\Delta L = (1 - \tau_{at}\tau_c)\Delta L_{cb}, \quad (2.52)$$

en donde $\Delta L_{cb} = B_c - L_b$.

Por lo tanto, el modelo de transferencia de radiación para la determinación del ILS es dado por la ecuación (2.52), con $\tau_{at} = 1$ debido a que la medición de la nube de gas se efectúa justo enfrente de la entrada del espectrómetro.

La figura 2.5 muestra la configuración experimental utilizada durante la determinación del ILS del espectrómetro OPAG 22 en donde se incluyó una fuente de radiación infrarroja, una celda de gas (de un paso óptico de 2 cm con ventanas de BaF₂) y el espectrómetro OPAG 22.

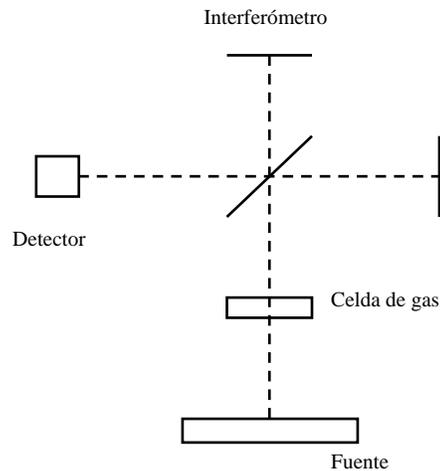


Figura 2.5 Diseño experimental de la medición del espectro de transmisión de CO: Cuerpo negro, celda de gas, y espectrómetro. Como gas se utilizó monóxido de carbono (CO) debido a su intensa absorción en el infrarrojo, baja o ausente concentración en la atmósfera (para así eliminar posibilidades de sobre estimación en su concentración) y a la presencia de sus parámetros espectroscópicos en la base de datos HITRAN (necesario para simular la transmisión/absorción de radiación).

El principio de medición está basado en que la radiación infrarroja, emitida por una placa metálica capaz de elevar la temperatura de su superficie a más de 200 C°, es absorbida por las moléculas activas en el infrarrojo presentes en el paso óptico de tal forma que son obtenidos espectros de absorción (L_{med}) que son aproximados a un espectro sintético (L_{model}) a través de la convolucion del espectro sintético con la función forma del instrumento.

Una vez caracterizado el espectro de absorción de CO en la región espectral que va de 2048 a 2058 cm^{-1} , el software GeDetekt fue utilizado para realizar el ajuste entre el espectro sintético y el espectro medido a través de la modificación de los cinco parámetros característicos de la ecuación 2.28 dando como resultado una ILS que presentó como particularidad el ensanchamiento de línea y el desfase observados previamente por Harig et al. (2004) en un espectrómetro OPAG 22 de menor resolución espectral (1 cm^{-1}). Como es de esperarse, los efectos de ensanchamiento y desfasamiento de línea en nuestro instrumento resultaron ser aún más pronunciados que los medidos por Harig debido a la diferencia mecánica (esta diferencia consiste en que uno de los brazos del interferómetro es unos milímetros mas largo que el otro) existente entre los interferómetros que nos permite obtener una resolución espectral máxima de 0.2 cm^{-1} .

2.3.3 Comparación de los resultados

En su versión original, el software MAPS tuvo incluido en su código fuente la función de apodización Norton Beer Strong (NBS) a través de la cual fue plasmada la influencia del espectrómetro K300 en los espectros sintéticos usados en el análisis cuantitativo. Esta función tiene la particularidad de ser una función de apodización simétrica con brazos laterales positivos en todos sus puntos.

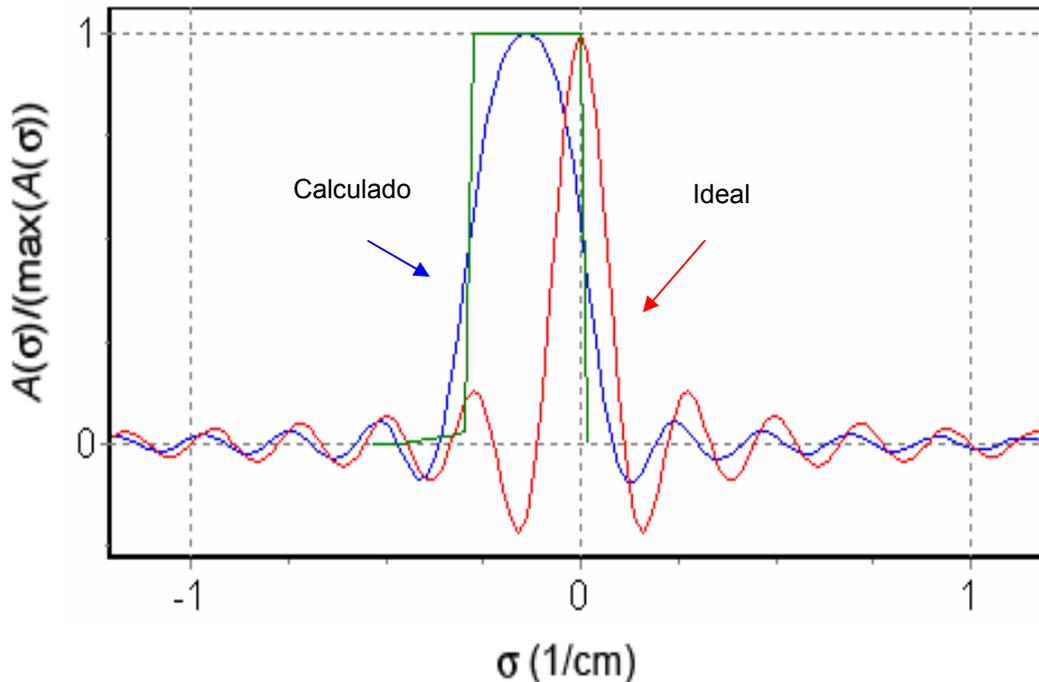


Figura 2.6. ILS ideal (rojo) y ILS medida (Azul) utilizando los espectros de CO calculado por el software GeDetekt.

Con el objetivo de observar el beneficio en el proceso de simulación de espectros utilizando la nueva función ILS, dos espectros de emisión infrarrojos medidos del escape de un turborreactor por el sistema SIGIS fueron simulados por MAPS utilizando como funciones de instrumento la nueva función ILS y la función original del software MAPS (con NBS).

Como resultado de la simulación, el coeficiente de correlación entre los espectros sintéticos y reales se incremento de 0.73 y 0.68, utilizando la función original del software MAPS (NBS), a 0.94 y 0.96 mostrando una mejoría significativa en el ajuste de fase e intensidad de línea.

Esto muestra claramente la importancia de esta función en la espectroscopía de emisión pues influye sistemáticamente la calidad de los resultados con lo cual se comprueba lo observado por los diferentes autores citados en esta sección.

En las mediciones presentadas en los siguientes capítulos, la función ILS del espectrómetro OPAG 22 mostrada en esta sección, será utilizada en el análisis cuantitativo realizado por MAPS .

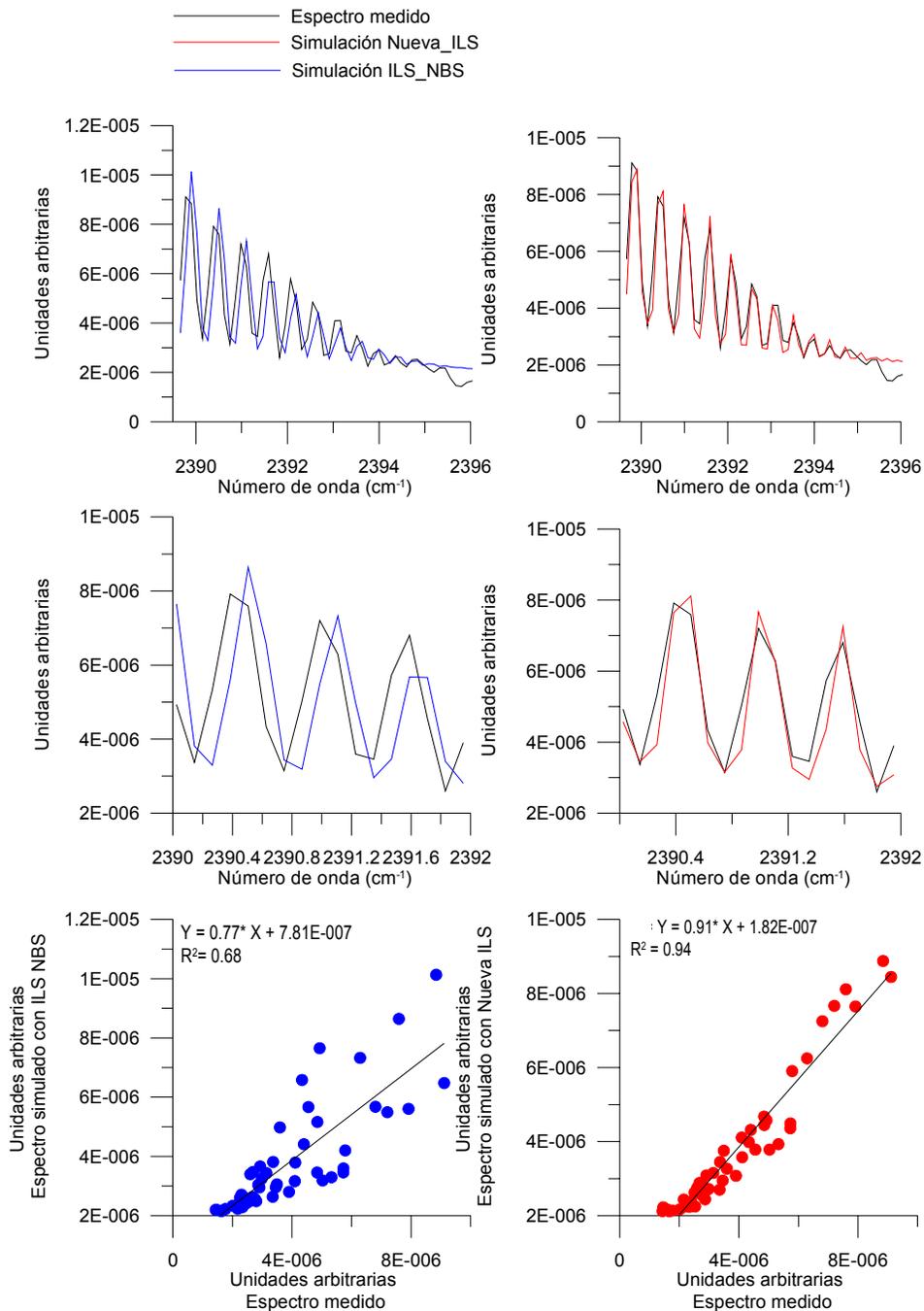


Figura 2.7. Esta figura muestra en la columna izquierda la simulación por MAPS de un espectro de emisión utilizando como ILS la función Norton Beer Strong y en la columna derecha la misma simulación pero en este caso utilizando la ILS calculada para el espectrómetro OPAG22.

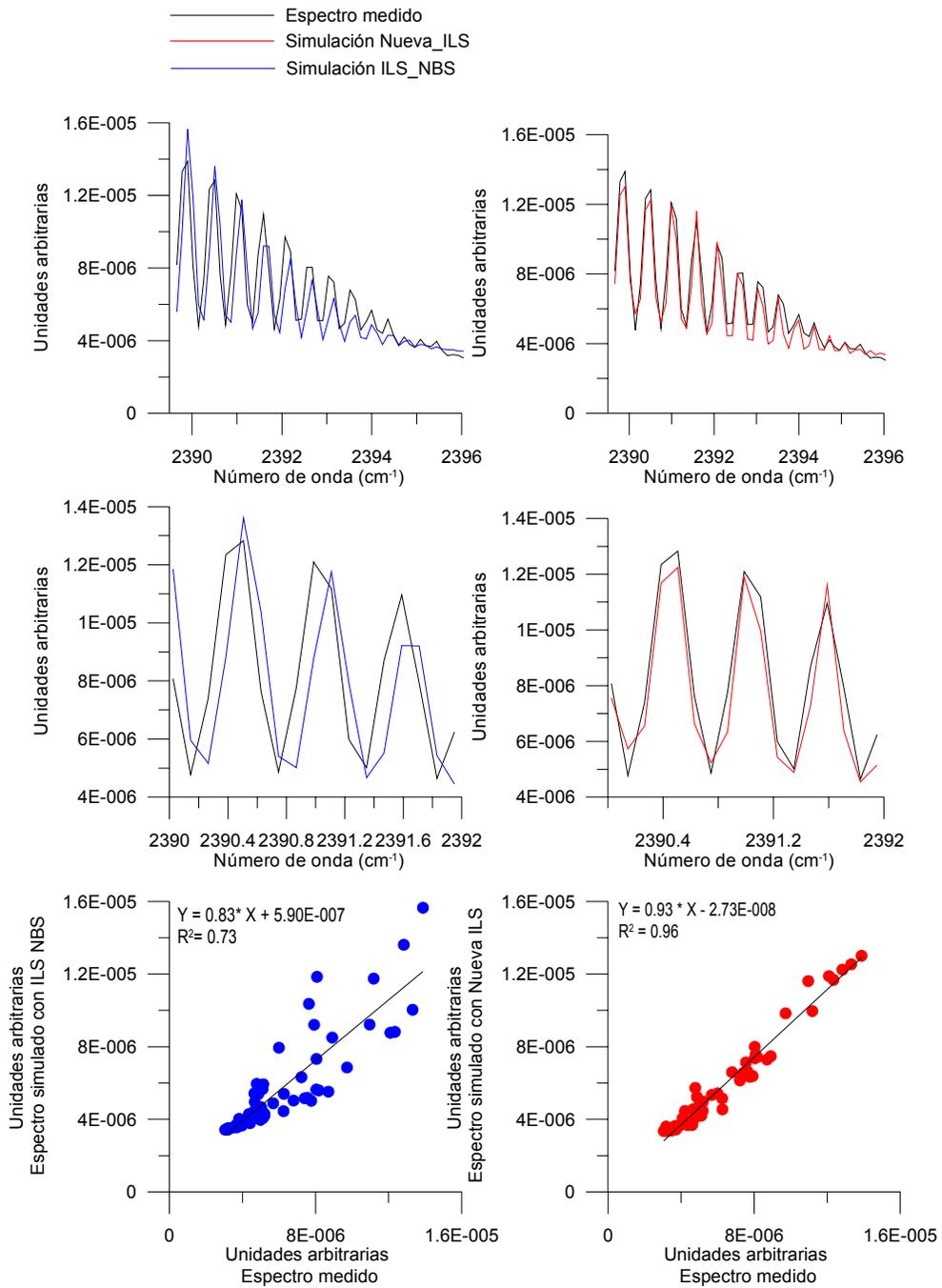


Figura 2.8. Esta figura muestra en la columna izquierda la simulación por MAPS de un espectro de emisión utilizando como ILS la función Norton Beer Strong y en la columna derecha la misma simulación pero en este caso utilizando la ILS calculada para el espectrómetro OPAG22.

3

EL SISTEMA DE VISUALIZACIÓN DE GASES EN EL INFRARROJO

3.1 El sistema SIGIS

El sistema de visualización de gases en el infrarrojo (SIGIS, por sus siglas en inglés) fue desarrollado originalmente con el objetivo de detectar y visualizar plumas de gases tóxicos (Harig et al., 2001, 2002 y 2004). Este sistema SIGIS está compuesto por un espectrómetro FTIR Bruker modelo Opag 22 con su telescopio, un espejo fijado a dos motores de pasos para el barrido bidimensional, una cámara infrarroja y un procesador y controlador del sistema (para el espectrómetro y el equipo de video) como se muestra en la figura 3.1.

El espectrómetro Bruker OPAG 22 incluido en el sistema SIGIS (Figura 3.2) tiene un rango de operación de 680 a 3500 cm^{-1} (con un detector MCT) y puede obtener espectros a baja resolución (56 cm^{-1}) con velocidades de 17 interferogramas por segundo y alta resolución (0.2 cm^{-1}).

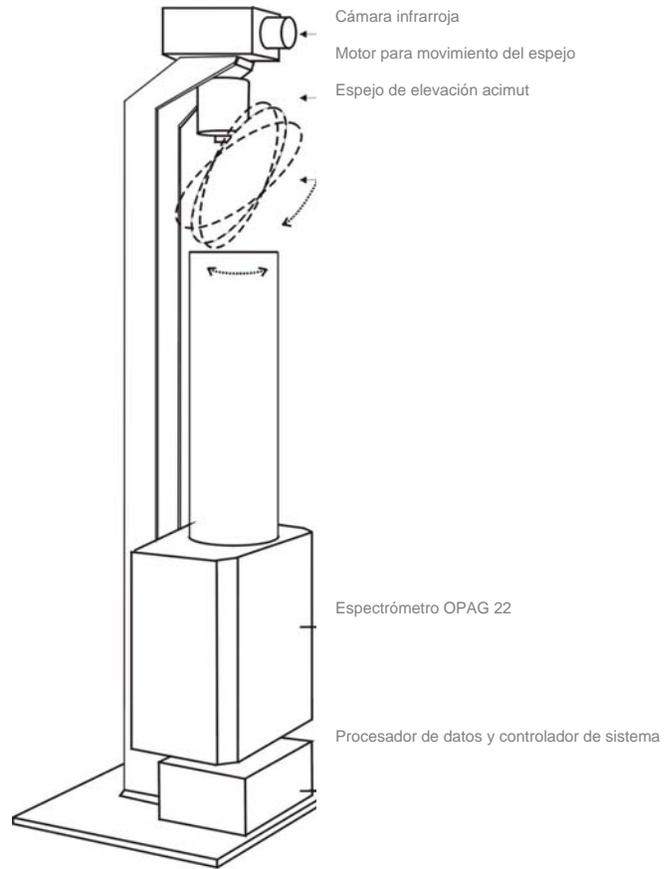


Figura 3.1 Esquema de componentes del SIGIS para la medición de la temperatura y la distribución de gases.



Figura 3.2. Esquema de componentes del espectrómetro OPAG 22 para la obtención de los espectros. BB. Cuerpo negro interno del espectrómetro, F; Espejo de 45°, I; interferómetro de doble péndulo, D; Detector MCT.

La figura 3.3 muestra en forma esquemática el funcionamiento de la obtención de espectros así como la interfase del sistema SIGIS. La cámara infrarroja al igual que el espectrómetro, son controlados por un procesador de datos y controlador de sistema (DSP), el cual manda la información, video y espectros, a una interfase escrita en C++ llamada GeDetekt.

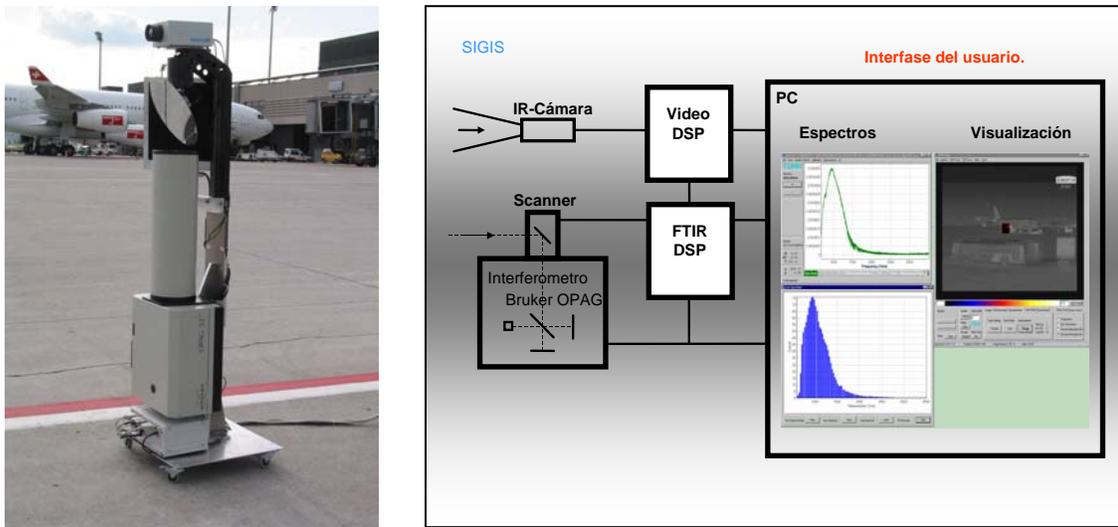


Figura 3.3 Izquierda: El equipo SIGIS en medición en el Aeropuerto internacional de Zurich. Derecha: Diagrama de bloque de la interfase del software GeDetekt.

3.2 Modo de operación

Para efectuar la visualización rápida del gas de escape de una turbina de avión se realiza un barrido bidimensional a lo ancho y largo de la pluma de emisión. En cada posición del barrido se colectan 17 interferogramas por segundo a baja resolución (56 cm^{-1}) y convertidos a espectros a partir de la transformada de

Fourier. Se calcula la temperatura de brillantez despejando T en la ecuación de Planck y usando el espectro medido. A partir de la función de temperatura de brillantez, se cuantifica una integral en un rango espectral que contiene líneas de emisión típicas de CO_2 ($2200\text{-}2300\text{ cm}^{-1}$). De igual forma, para evaluar la temperatura de fondo, el espectro es analizado en el rango espectral $800\text{-}1200\text{ cm}^{-1}$. Posteriormente, el software asigna colores falsos a cada píxel de las posiciones medidas con base en el resultado cuantitativo de la integral del área espectral en cuestión. Este proceso de visualización de plumas de gas es conocido como escaneo rápido de temperatura. Debido a que el objetivo es localizar cualitativamente las partes más calientes de la pluma de gas en el campo de visión, no es requerida una calibración radiométrica en esta etapa.

Una vez que la distribución espacial del gas es conocida, el próximo paso es coleccionar espectros a alta resolución (0.2 cm^{-1}) en la posición en donde la emisión de CO_2 es más alta. Para esto, al menos 30 espectros son coleccionados y promediados para alcanzar una relación señal-ruido satisfactoria. Los espectros a alta resolución son calibrados con un cuerpo negro colocado próximo al instrumento. La Figura 3.4 ilustra el procedimiento para la obtención de espectros evaluados posteriormente por el software MAPS.

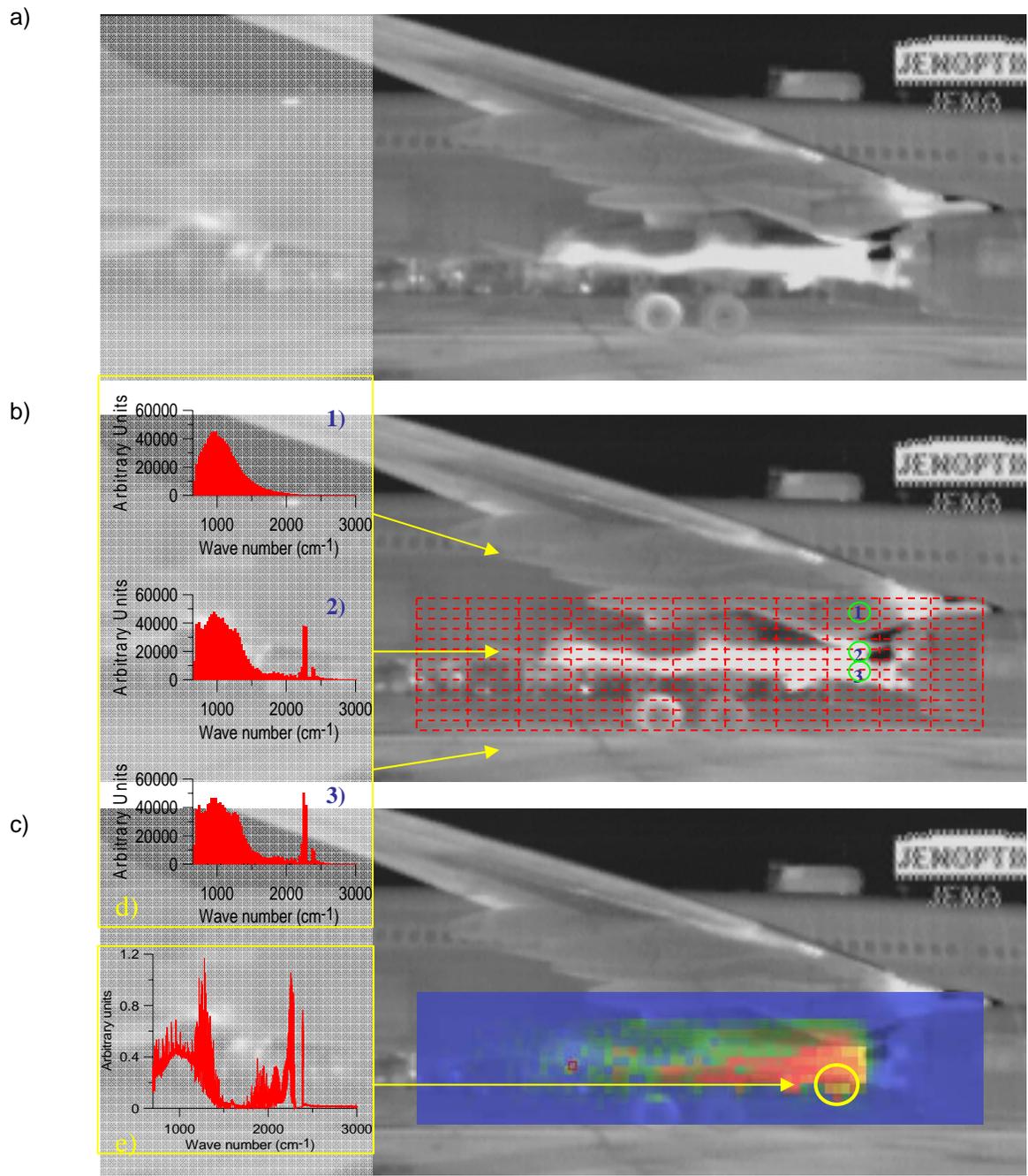


Figura 3.4 Procedimiento para la obtención de espectros a alta resolución con el sistema de visualización. Columna derecha: a) imagen térmica, b) área propuesta para realizar un barrido, c) colores falsos asignados debido a la información de los espectros colectados a baja resolución. Columna izquierda: c) Tres espectros a baja resolución colectados en el área rectangular de líneas entrecortadas. d) Espectro a alta resolución en la posición de más alta temperatura encontrada dentro del campo de visión.

CAPÍTULO

4

TÉCNICAS DE VALIDACIÓN PARA EL FTIR
PASIVO

Autores como Griffiths et al. (1999) han estimado de experimentos en celda de gas que la incertidumbre en la determinación de la concentración de moléculas como CO₂ y NO₂ por la técnica FTIR en configuración activa es del rango de ~3%. Las principales fuentes de incertidumbre en esta configuración se le atribuye al desconocimiento exacto de la longitud del paso óptico dentro de la celda de gas, a la pureza de los gases de calibración (la incertidumbre en la preparación de gases estándares por gravimetría es ~0.002 μmol/mol (ppm)) y a la base de datos moleculares HITRAN (2%). HITRAN es utilizada por el módulo LBL para la creación de espectros sintéticos posteriormente ajustados a un espectro medido.

El escenario es diferente cuando se realizan mediciones con la espectroscopia infrarroja en configuración pasiva. En ésta técnica de medición, los niveles de incertidumbre han sido estimados al rededor del 30% por Heland et al. (1997) siendo la conversión de datos moleculares a altas temperaturas la fuente de incertidumbre más importante. La incertidumbre en los datos moleculares proporcionados por la base de datos HITEMP es de hasta ~15% dependiendo

de la especie. También se suman a ésta el ancho del rango espectral para el cálculo LBL y la incertidumbre en la función ILS del instrumento. Es por tanto importante contar con un arreglo experimental a partir del cual se pudieran mediante condiciones controladas, comparar los resultados obtenidos con las mediciones en configuración pasiva y así estimar las incertidumbres.

Como parte de este trabajo, se investigaron dos arreglos instrumentales; un quemador diesel con el cual Heland et al. (1997) realizaron la evaluación de sus resultados con el espectrómetro K300, y una celda de gas diseñada y producida durante el proyecto AEROTEST.

En este capítulo se muestra en detalle, tanto el desarrollo experimental como los resultados obtenidos, de ambos arreglos experimentales. En ambos casos se obtiene una incertidumbre similar a la reportada por Heland et al. (1997) de 30% debido a que ésta es principalmente originada en la cuantificación de los resultados provenientes del cálculo de los espectros sintéticos.

4.1 Quemador diesel

4.1.1 Instrumentación

El arreglo instrumental del quemador diesel consistió en un quemador comercial, normalmente utilizado para uso industrial, con una potencia de 356kW. Éste fue acoplado a un tubo de acero inoxidable de 50 cm de diámetro acondicionado con un ventilador el cual es capaz de generar un flujo de 40,000 L/min de gas. (Ver figura 4.1a)

En la figura 4.1b se muestra la configuración de la medición simultánea llevada a cabo con los instrumentos K300 y SIGIS. Ambos fueron situados a una distancia de 9 metros del quemador, el campo de visión del espectrómetro K300, fue situado directamente detrás de la boquilla del quemador de tal forma que las mediciones de la pluma de gas realizadas con este espectrómetro se efectuaron en una sola posición. El campo de visión del sistema SIGIS fue utilizado para efectuar el procedimiento FTS (capítulo 3) directamente detrás de la boquilla de salida con el objetivo de caracterizar la distribución de la temperatura dentro de la pluma de gas. Posteriormente fueron colectados espectros a alta resolución (0.2 cm^{-1}) en diferentes zonas de la pluma de gas y en diversas secuencias de medición (descritas en la siguiente sección) en las que se inyectaron dentro del quemador gases de calibración (CO y NO) con el objetivo de magnificar la señal

de estas especies y utilizarlas como trazadores del comportamiento de los gases dentro de la corriente de escape del quemador.

4.1.2 Mediciones

La secuencia de medición llevada a cabo con el espectrómetro K300 y el sistema SIGIS es enlistada a continuación:

Espectrómetro K300.

- 22 espectros en una sola posición en paralelo con el sistema SIGIS.

Sistema SIGIS.

- Mediciones en 11 posiciones en paralelo con el espectrómetro K300 en secuencia vertical,
- Mediciones en 11 posiciones con inyección del gas CO en secuencia vertical,
- Mediciones en 25 posiciones para la determinación de los cambios de concentración y temperatura de los gases de escape con respecto a la distancia de la salida del quemador en secuencia vertical y horizontal.

4.1.3 Resultados

Con el objetivo de caracterizar el perfil vertical de la temperatura de los gases de escape, se realizó el procedimiento FTS de los gases de salida del quemador (figura 4.1 c y d) a través del cual se observó una distribución no-homogénea de la temperatura dentro de la pluma de gas. Este fenómeno es un resultado importante debido a que en las mediciones realizadas para la validación de resultados con el espectrómetro K300 (Heland, 1997), pudieron haberse realizado mediciones en zonas en las que pudieron haber coexistido grandes diferencias de temperatura y concentración de gas afectando así la evaluación de resultados.

Con la finalidad de cuantificar el grado de discrepancia de la temperatura en dos zonas diferentes dentro de la pluma de gas, se eligieron dos posiciones en la pluma de salida de acuerdo al grado de contraste en color que estas tuvieron (figura 4.1 c y d). De estas posiciones, espectros a alta resolución fueron colectados. Como resultado, la diferencia en temperatura calculada a partir de los espectros fue de hasta $100\pm 30^{\circ}\text{C}$.

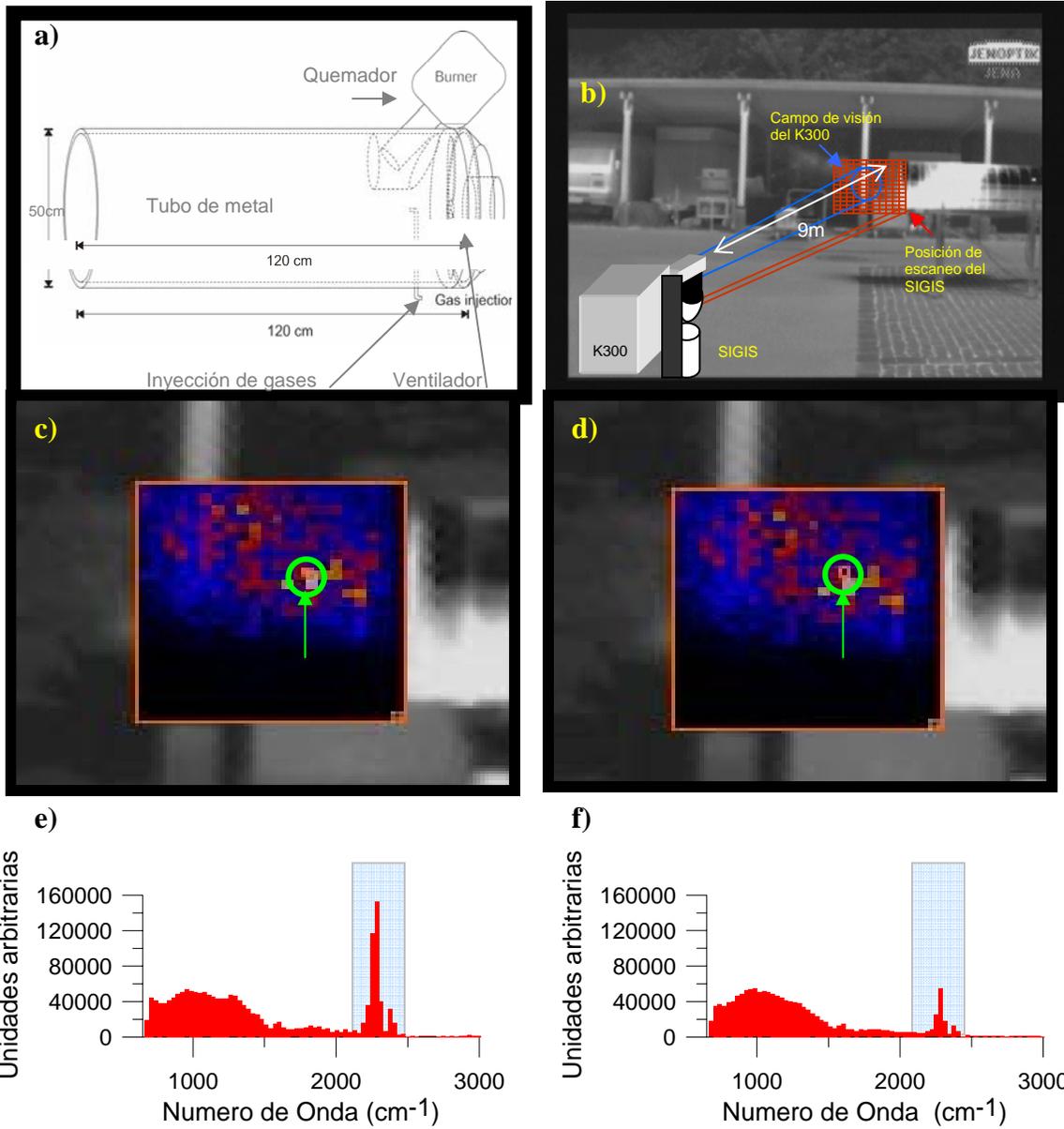


Figura 4.1 a) Esquema de construcción y dimensiones del quemador a diesel. b) Imagen infrarroja del quemador en el cual se muestra el campo de visión del espectrómetro K300 y el área de escaneo del sistema SIGIS. c y d) posiciones elegidas para la obtención de espectros a alta resolución. e) y f) espectros a baja resolución (56 cm^{-1}) correspondientes a las posiciones de la fig. c y d.

4.1.3.1 Comparación de resultados entre el sistema SIGIS y el espectrómetro K300

Con el objetivo de comparar los resultados, se llevaron a cabo mediciones con el espectrómetro K300 y el sistema SIGIS en forma paralela y simultánea. Con el espectrómetro K300 se colectaron 22 espectros a alta resolución en una sola posición y con el sistema SIGIS se colectaron 12 espectros en la vertical con un intervalo entre cada posición de medición de ~ 3 cm y un tiempo de adquisición de 60 segundos para cada espectro (Figura 4.2).

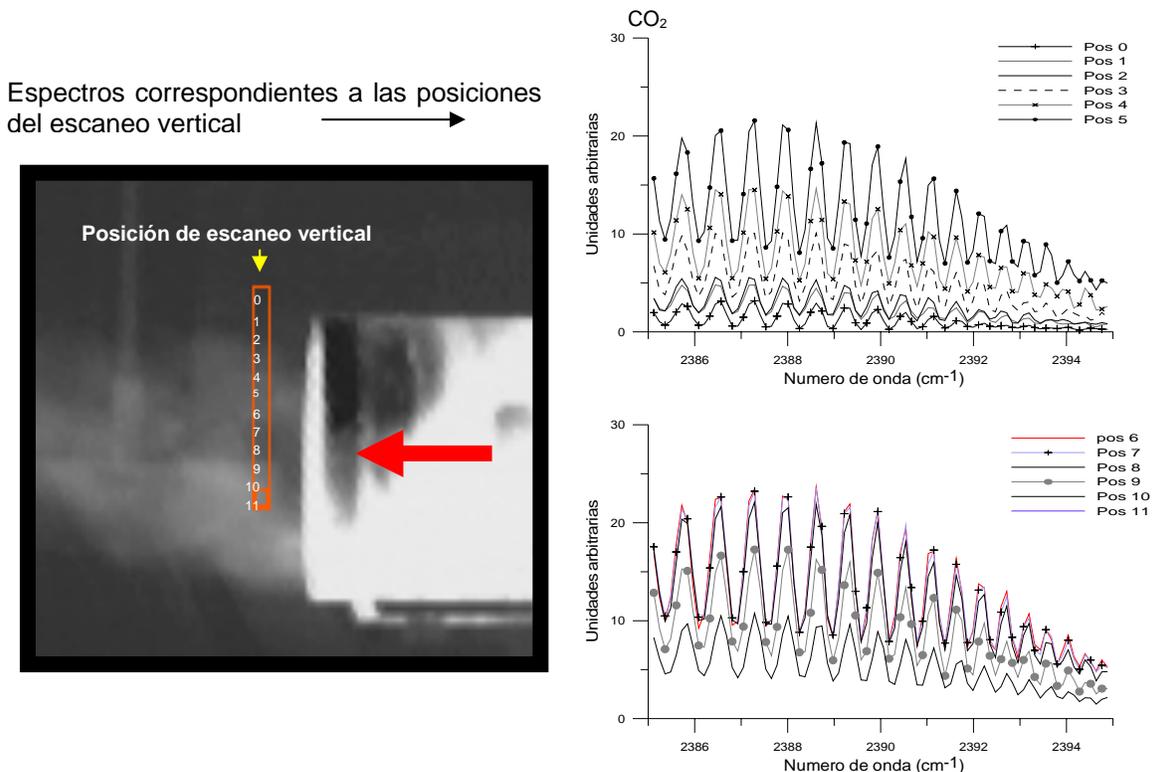


Figura 4.2 Izquierda: Imagen infrarroja del quemador en operación durante la medición de 12 espectros. Derecha: Espectros a alta resolución (0.2cm^{-1}) no calibrados graficados en la región típica de la emisión de CO_2 en donde puede observarse que las líneas de emisión del CO_2 en la región $2385\text{-}2395\text{cm}^{-1}$ presentan importantes diferencias en intensidad y forma de acuerdo a la posición en donde fueron obtenidas. Las líneas de emisión presentan una débil señal para la posición 0 y señales muy intensa y claras para las posiciones 5 y 6.

En la figura 4.3 se muestra el resultado del cálculo de temperatura por ambos equipos. En puntos rojos se muestran los resultados medidos por el espectrómetro K300 y en puntos negros, los valores de concentración obtenidos por el sistema SIGIS en las doce posiciones. En esta puede apreciarse que la variación temporal y espacial de la temperatura y concentración tiene aproximadamente la misma magnitud, pues los valores de temperatura están dentro del rango de incertidumbre de la medición.

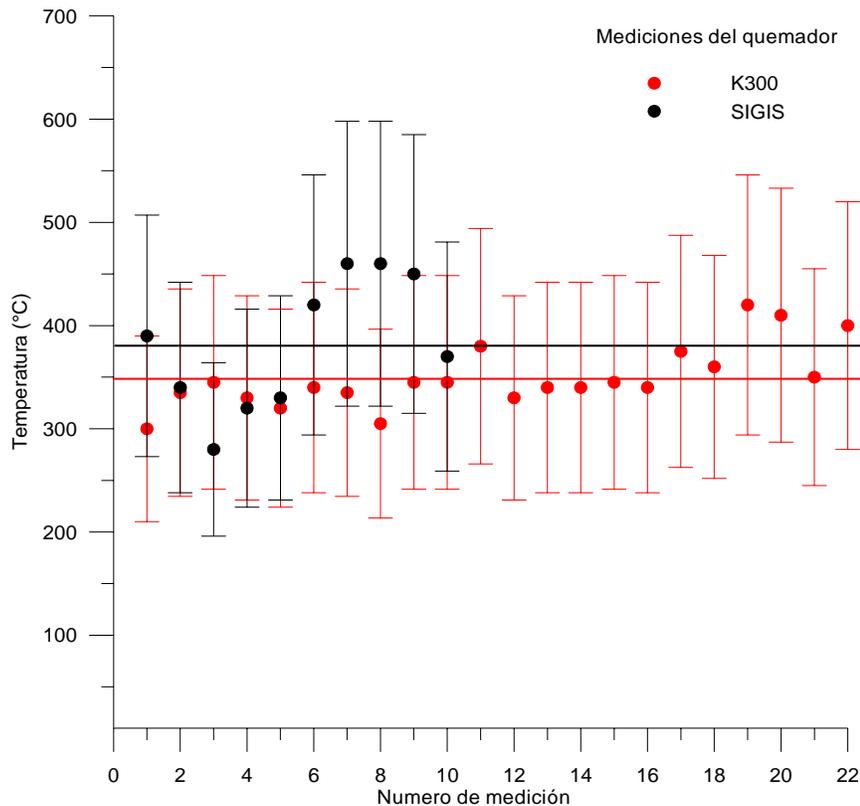


Figura 4.3 Comparación de resultados del espectrómetro K300 y el sistema SIGIS. En ellos se puede ver la consistencia en los valores de temperatura dados por ambos sistemas a pesar de que la mejor estimación de temperatura, en algunas posiciones, no fue muy similar esta cae dentro del rango de incertidumbre de ambos sistemas. Las líneas continuas representan el promedio de temperaturas en ambos casos.

La figura 4.4 muestra los gráficos de comparación de resultados de concentración obtenidos por el sistema SIGIS y el espectrómetro K300 de los compuestos CO, CO₂ y H₂O. En éstos, al igual que en los resultados de temperatura, puede observarse consistencia en los resultados de concentración reportados por ambos sistemas. La concentración promedio reportada por el sistema SIGIS y por el espectrómetro K300 fue de $3.07 \pm 0.92 \times 10^{+18}$ moléculas por cm² y $3.68 \pm 1.10 \times 10^{+18}$ moléculas por cm², respectivamente. (La posiciones 0 y 11 no pudieron ser computadas debido a la baja intensidad en señal). Debido a la baja concentración de NO emitido por el quemador, el sistema SIGIS no pudo determinar el perfil de concentración de éste compuesto, sin embargo la sección 4.1.3.3 óxido nítrico a alta concentración fue inyectado dentro del quemador.

Tabla 4.1. Promedio de temperatura y concentración del sistema SIGIS y del espectrómetro K300.

	Temperatura	CO₂	CO	H₂O
	°C	(moléculas por cm ²)	(moléculas por cm ²)	(moléculas por cm ²)
<i>SIGIS</i>	382±104	3.07±0.92E+18	7.23 ±2.16E+16	5.67±1.70E+18
<i>K300</i>	349±114	3.68±1.10E+18	7.42 ±2.22E+16	6.94±2.08E+18

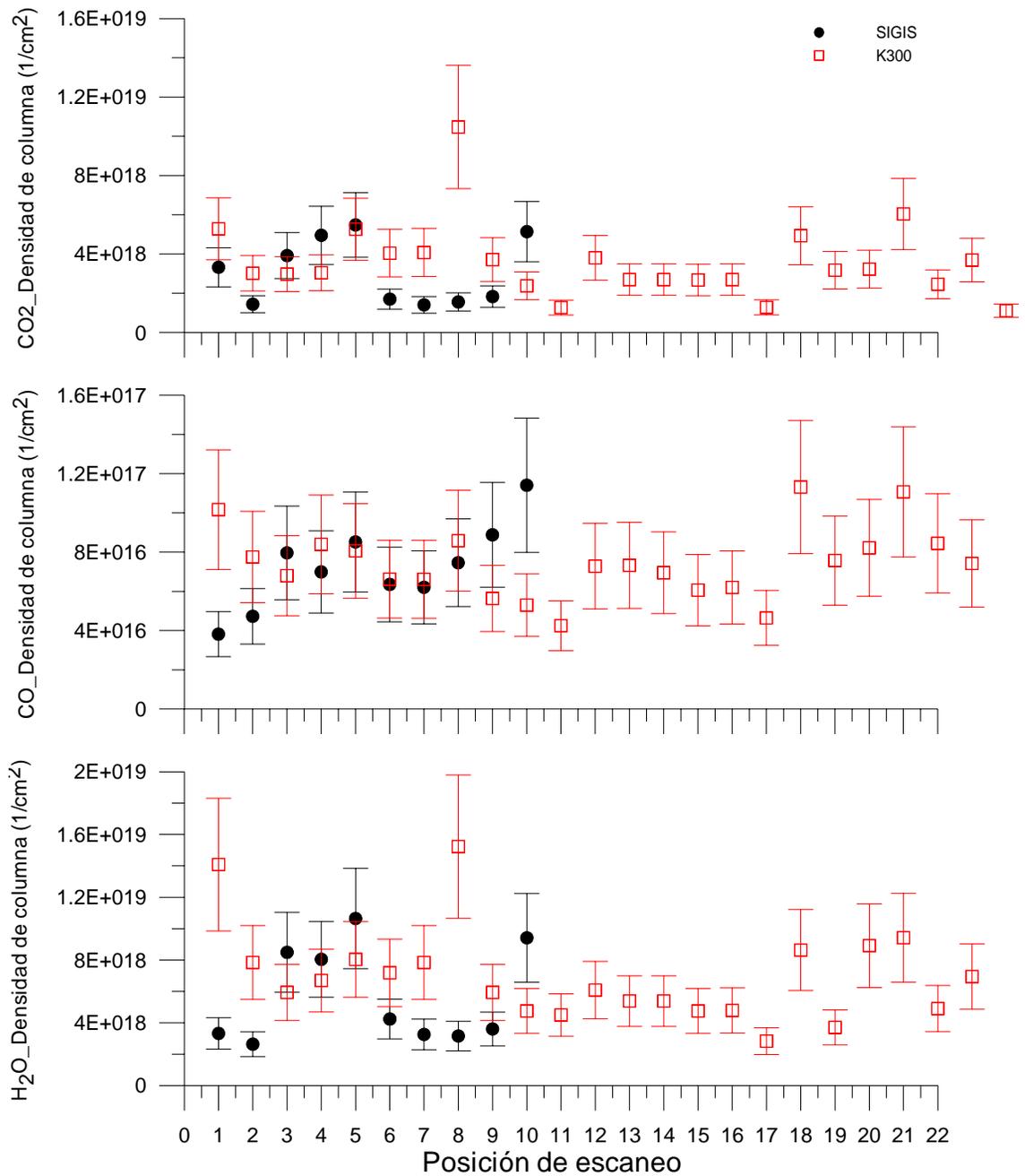


Figura 4.4. Distribución espacial de densidad de columna de los gases a)CO₂, b)CO y c) H₂O obtenidos por MAPS utilizando espectros del sistema SIGIS y el espectrómetro K300. Las Barras de error corresponden a una incertidumbre del 30% en ambos casos. Nótese que en las posiciones de escaneo número 3,4 y 5 (que justo el medio de la pluma) las mediciones reportadas por el SIGIS son consistentes.

4.1.3.2 Inyección de monóxido de carbono dentro del quemador.

Con el objetivo de magnificar la señal de monóxido de carbono y observar el cambio en la concertación de salida del CO y CO₂, se inyectaron dentro del quemador 1000 ppmV de este gas. La siguiente figura (4.5) muestra los espectros de emisión colectados antes y después de la inyección de éste gas.

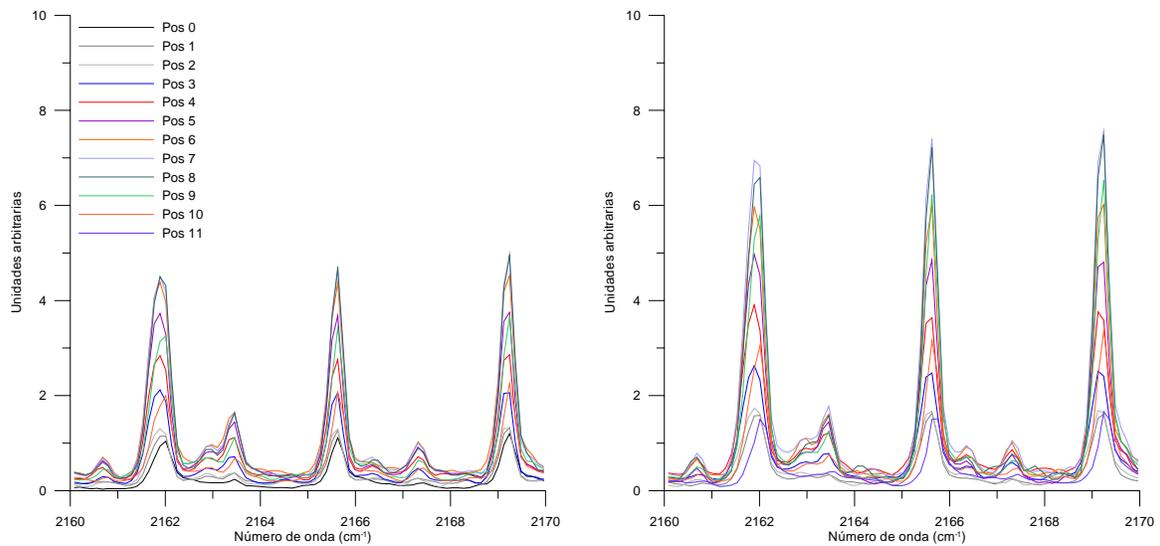


Figura 4.5. Espectros a alta resolución (0.2cm^{-1}) no calibrados graficados en la región típica de la emisión de CO, en donde se puede observar el incremento de la señal en las líneas de emisión de CO, región $2166\text{-}2175\text{cm}^{-1}$, antes (espectros del lado izquierdo) y después de la inyección de CO. Note el cambio de escala en el eje Y.

Se realizó nuevamente la medición de los gases emitidos en la misma configuración de la sección anterior con la finalidad de localizar la posición en la pluma de gases de salida en la cual se concertó la mayor cantidad de este gas. Como resultado del análisis cuantitativo de los espectros de emisión, se observó que el perfil de temperatura obtenido a través de ambas mediciones fue similar, sin embargo, la temperatura en las posiciones 1,2 y 5 presento pequeñas

diferencias respecto al perfil anterior a la inyección de gases que se encontró dentro del rango de incertidumbre de la medición (ver figura 4.6). El promedio de temperatura obtenido en ambos casos fue de $382 \pm 114^\circ\text{C}$ y $373 \pm 111^\circ\text{C}$ antes y después de la inyección del gas respectivamente. La concentración de CO_2 se mantuvo estable posterior a la inyección ($3.07 \pm 0.92 \times 10^{+18}$ y $2.99 \pm 0.89 \times 10^{+18}$ moléculas por cm^2). Como era de esperarse, la concentración de CO aumento en 64% al pasar de $7.23 \pm 2.16 \times 10^{+16}$ á $1.19 \pm 0.35 \times 10^{+17}$ moléculas por cm^2 confirmándose así la identificación del cambio de concentración del gas observado fuertemente en las posiciones 1,2 y 3 .

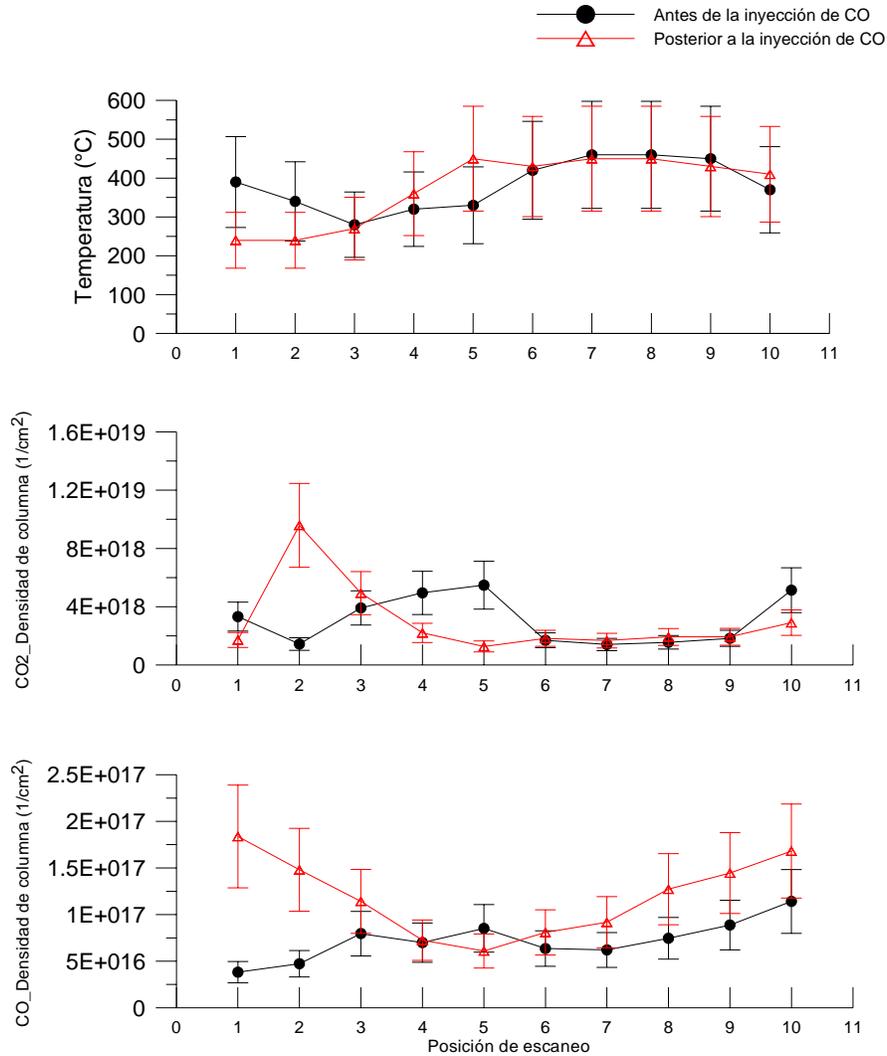


Figura 4.6. Esta figura muestra la distribución espacial de a) temperatura y densidad de columna de los gases b) CO₂ y c) CO obtenida por el sistema SIGIS en un escaneo vertical en 12 posiciones. Las Barras de error corresponden a una incertidumbre del 30%.

4.1.3.3 Inyección de óxido nítrico dentro del quemador.

Debido a la baja emisión de este compuesto en la pluma de gas de quemador se inyectó a este equipo 10 L/min de NO (con una pureza del 99%). A diferencia de la medición anterior, en esta ocasión se empleó una nueva configuración para la obtención de los espectros de emisión la cual consistió en la obtención de

espectros en dirección vertical y horizontal, (como se ilustra en la figura 4.7) con el objetivo de obtener un perfil de temperatura y concentraciones más completo.

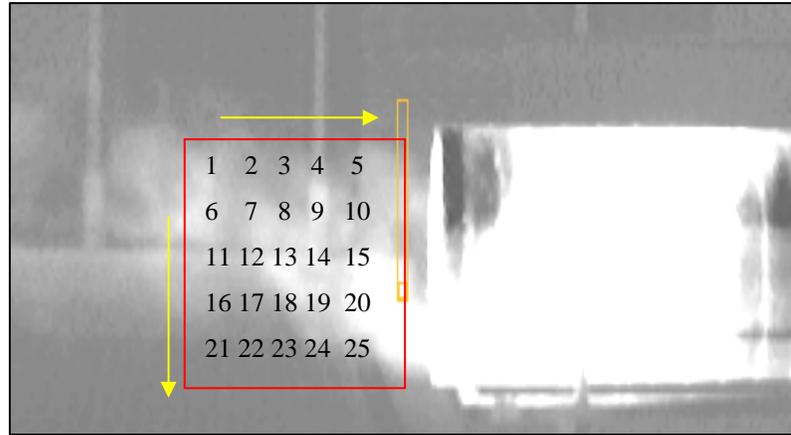


Figura 4.7 Imagen infrarroja del quemador en operación durante la medición de espectros. El área dentro del recuadro de línea roja establece la posición de medición de cada espectro correspondiente a cada píxel.

Como resultado de la medición se obtuvieron 20 de los 25 espectros planeados originalmente (figura 4.8) debido a problemas técnicos con el quemador (obstrucción de un inyector de combustible). Los 20 espectros obtenidos presentaron en su totalidad una señal muy clara e intensa en la región característica del NO (1900.3cm^{-1}).

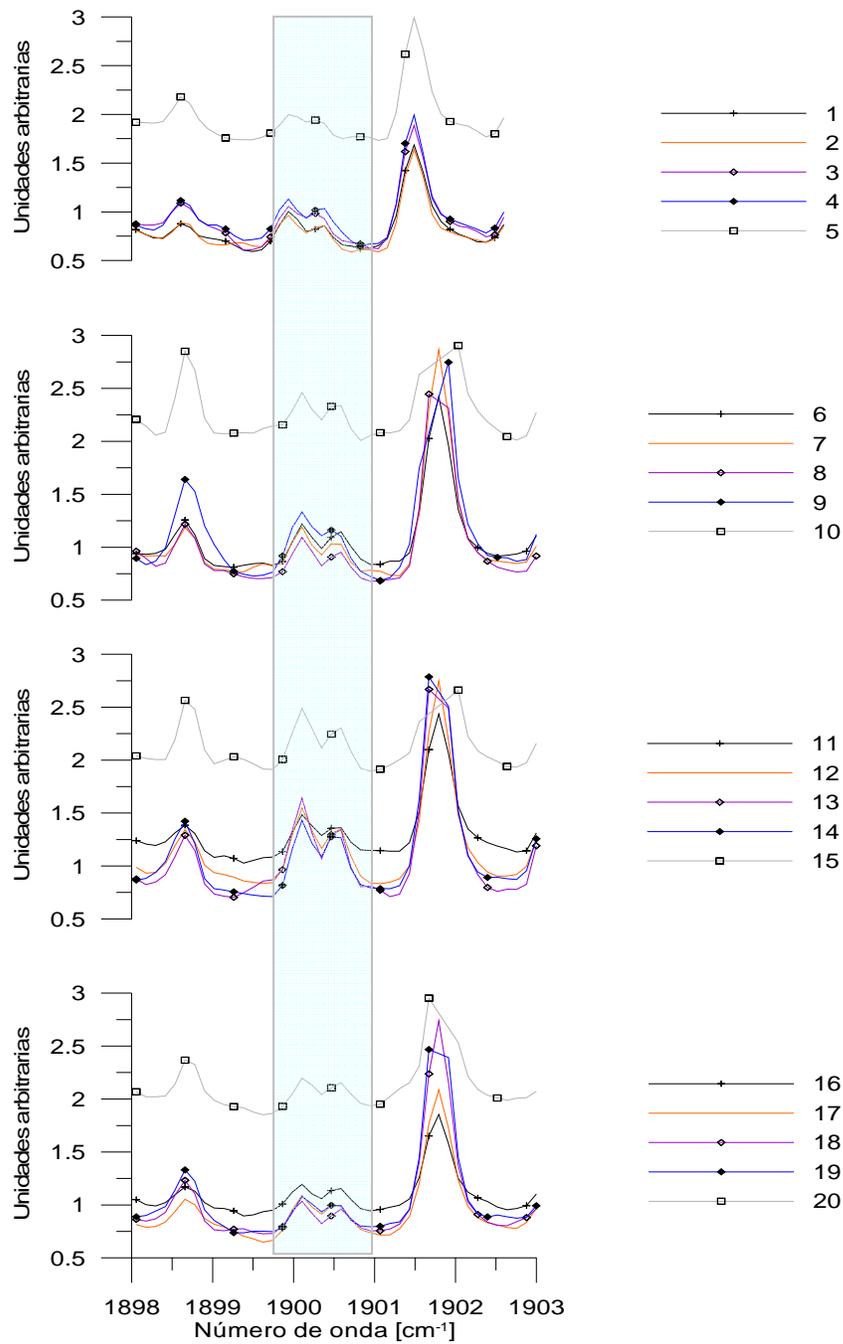


Figura 4.8. Espectros infrarrojos, no calibrados a alta resolución (0.2cm^{-1}), graficados en la región típica de NO, obtenidos durante la inyección de 10 L/min. de NO dentro del quemador. Nótese la intensidad de la doble línea de emisión de este gas ubicada en la región 1900.0 a 1901cm^{-1} debido a la presencia de la alta concentración de este gas dentro de la pluma.

La figura 4.9 muestra el perfil corriente abajo de temperatura (en la cual no se incluyó el valor de incertidumbre por razones de estética en la imagen) de la pluma de gas en donde puede observarse el enfriamiento del gas al mezclarse con el aire del entorno.

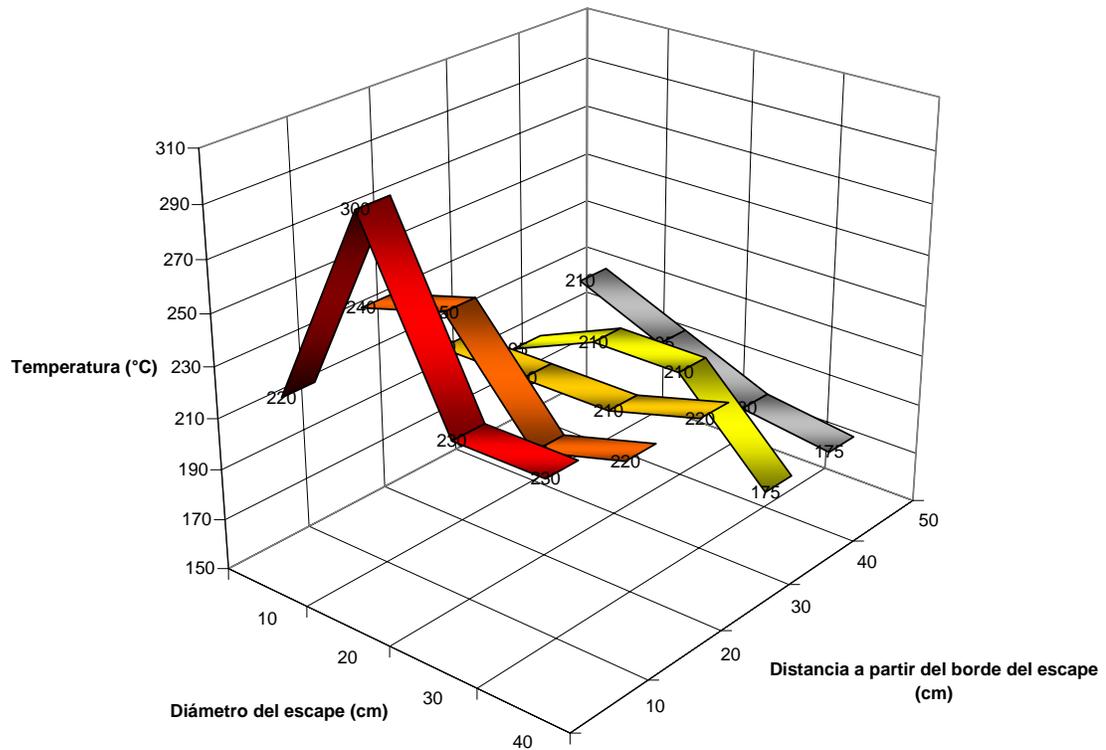


Figure 3.9. Gráfico de la distribución espacial de temperatura de los gases de escape del quemador en donde se aprecia la asimetría en la distribución de la temperatura.

La asimétrica en la distribución de la temperatura de la pluma de gas se hizo evidente en este tipo de gráfico. La figura 3.10 muestra la distribución de CO y NO dentro de la corriente de gases de escape, respectivamente.

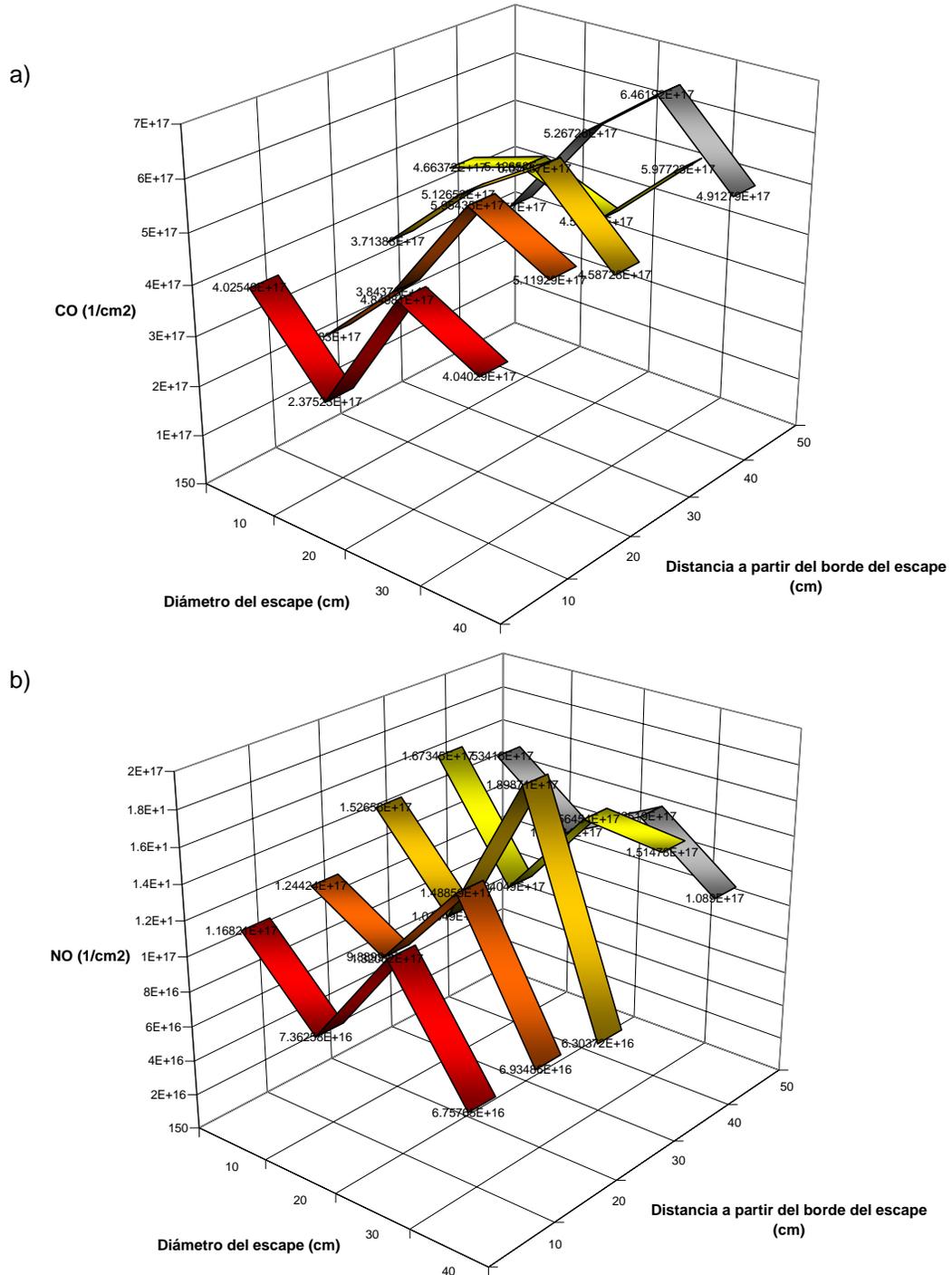


Figure 3.10. Distribución espacial de densidad de columna de los gases CO(c) y NO (d) dentro de la corriente de escape. Por razones de practicidad y estética de las imágenes no fueron incluidos los rangos de incertidumbres en las mediciones (30%).

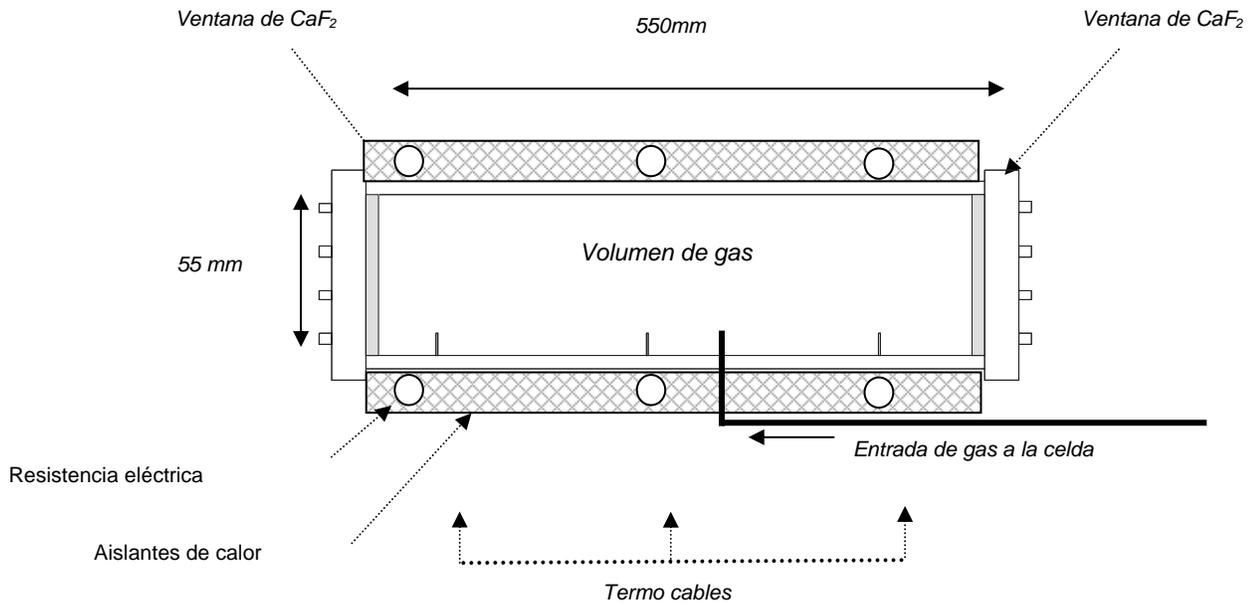
En el gráfico de distribución espacial de NO, figura 3.10 b), puede observarse que la densidad de columna de éste gas es mayor a razón que se incremente la distancia con respecto a la boquilla del quemador debido la deficiente mezcla de los gases a la salida. Como conclusión general de este experimento puede afirmarse que el quemador comercial utilizado por Heland et al. (1997) sí ofrece una corriente de gas rica en CO, CO₂ y H₂O (no así en monóxido de nitrógeno) pero éste presenta problemas técnicos muy importantes para la generación de una corriente de gas estable, lo cual resulta ser prioritario para un equipo de validación de resultados.

4.2 Celda de gases caliente

4.2.1 Instrumentación

La celda de gas, investigada como segundo equipo de comparación de resultados, fue construida en acero inoxidable y cuenta con ventanas de fluoruro de calcio, transparentes a la región infrarroja media 500 a 2500 cm⁻¹. La celda de gas cuenta con un módulo de monitoreo y control de temperatura que incluye tres indicadores individuales de temperatura, correspondientes a tres termopares colocados en el medio y los extremos de la celda y una camisa de calentamiento envolvente que tiene la capacidad de elevar la temperatura de la celda de gas hasta 500°C. El paso óptico de la celda de gas es de 550 mm y el diámetro de

las ventanas, así como del cilindro en donde los gases son confinados, es de 55 mm (ver figura 3.12).



4.11. Sección transversal de la celda de gas.

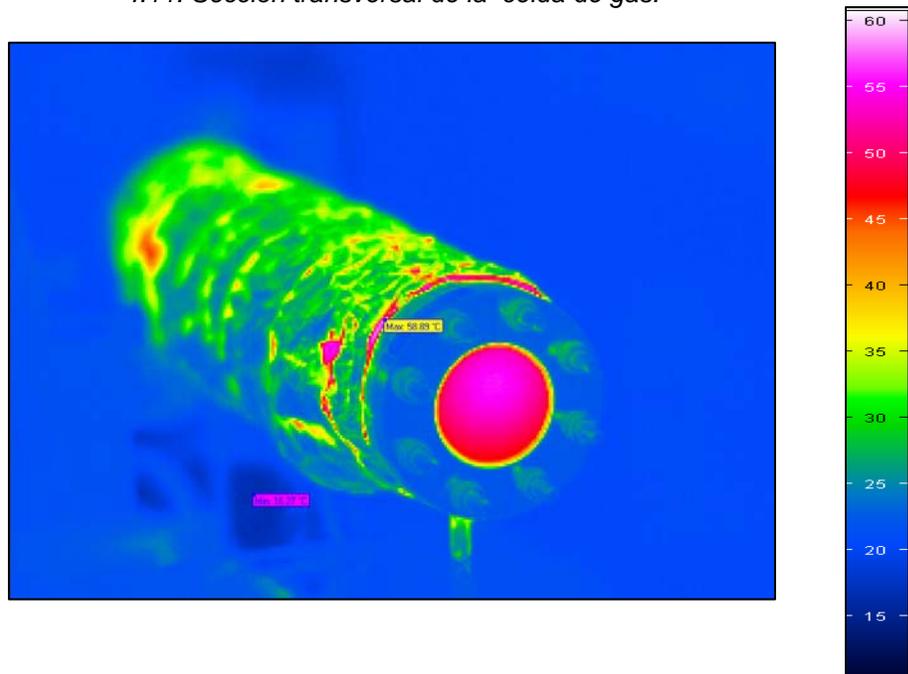
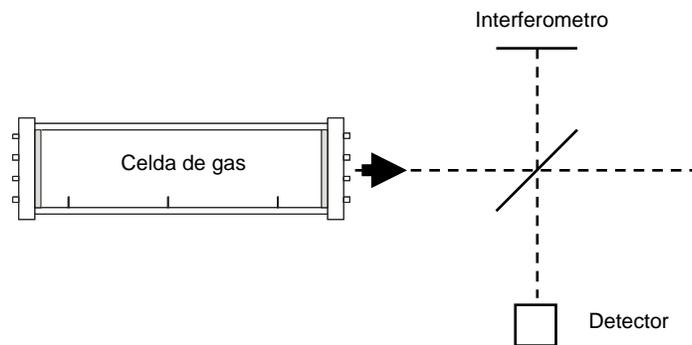


Figura 4.12. Imagen infrarroja de la celda de gas en operación durante la medición. La figura muestra en tonos rojizos las áreas más calientes de la celda de gas (60°C) y en azules las áreas relativamente más frías durante la estabilización térmica de la celda de gas previo a su uso. Nótese las fugas de calor del aislante térmico en tonos rojos.

4.2.2 Arreglo Experimental.

El dibujo esquemático de la figura 4.13 ilustra la configuración utilizada durante la medición. El espectrómetro OPAG22 fue desmontado de la base del sistema SIGIS (ver figura 3.1 del capítulo 3) y posicionado frente a la celda de gas con la finalidad de captar la radiación infrarroja emitida por los gases a alta temperatura confinados dentro de ésta.



4.13. Diseño experimental para la medición de los espectros de emisión de una mezcla de gases por celda de gas.

La celda de gas fue operada en un rango de temperatura de 200 á 450°C para lo cual fueron requeridos lapsos de 30 minutos de estabilización térmica del sistema para cada uno de los rangos de temperatura.

Posterior al procesos de estabilización térmica, la celda de gas fue evacuada en cinco ocasiones (por medio de una bomba de vacío) y llenada con nitrógeno de alta pureza antes de introducir la muestra de gases a caracterizar. Una vez realizado este procedimiento la mezcla de gases fue evacuada e introducida también en cinco ocasiones. El gas utilizado para la medición fue una mezcla

aire sintético, dióxido y monóxido de carbono al 3.5% y 500ppmV respectivamente. La pureza del gas fue certificada con una incertidumbre extendida del 2% según el fabricante del gas (Air Liquide).

4.2.3 Mediciones y resultados

Tres series de mediciones fueron realizadas a cinco diferentes niveles de temperatura, 200, 250, 300, 350 y 400°C. La figura 4.14 muestra los espectros de emisión correspondientes a una de las series en la que pueden observarse diferencias importantes en intensidad y forma de líneas de cada espectro en relación a la temperatura del gas.

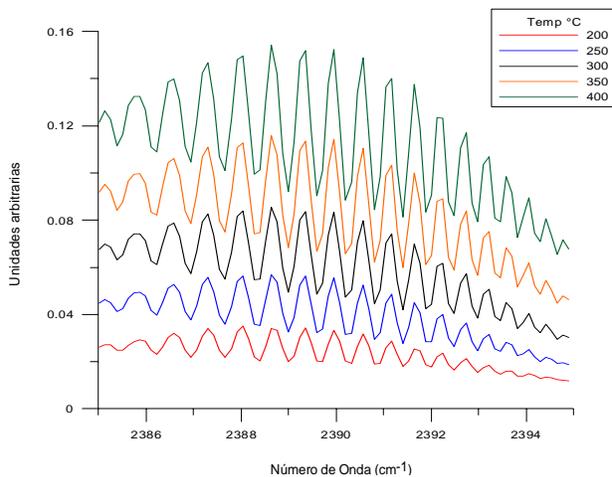


Figura 4.14. Espectros infrarrojos, no calibrados a alta resolución (0.2cm^{-1}), graficados en la región típica de CO_2 , obtenidos durante la medición de la mezcla de gases a cinco diferentes temperaturas (200, 250, 300, 350, 400). . En la figura puede observarse una clara diferencia en estructura e intensidad en cada uno de los espectros medidos.

Como resultado del análisis cuantitativo de los 15 espectros de emisión medidos por el espectrómetro OPAG 22, fue observado que la discrepancia entre los valores de temperatura dados por los indicadores de temperatura de la celda de

gas y los resultados obtenidos por MAPS, aumentó con el incremento en temperatura del gas dentro de la celda de gas linealmente (ver figura 4.15 y 4.16).

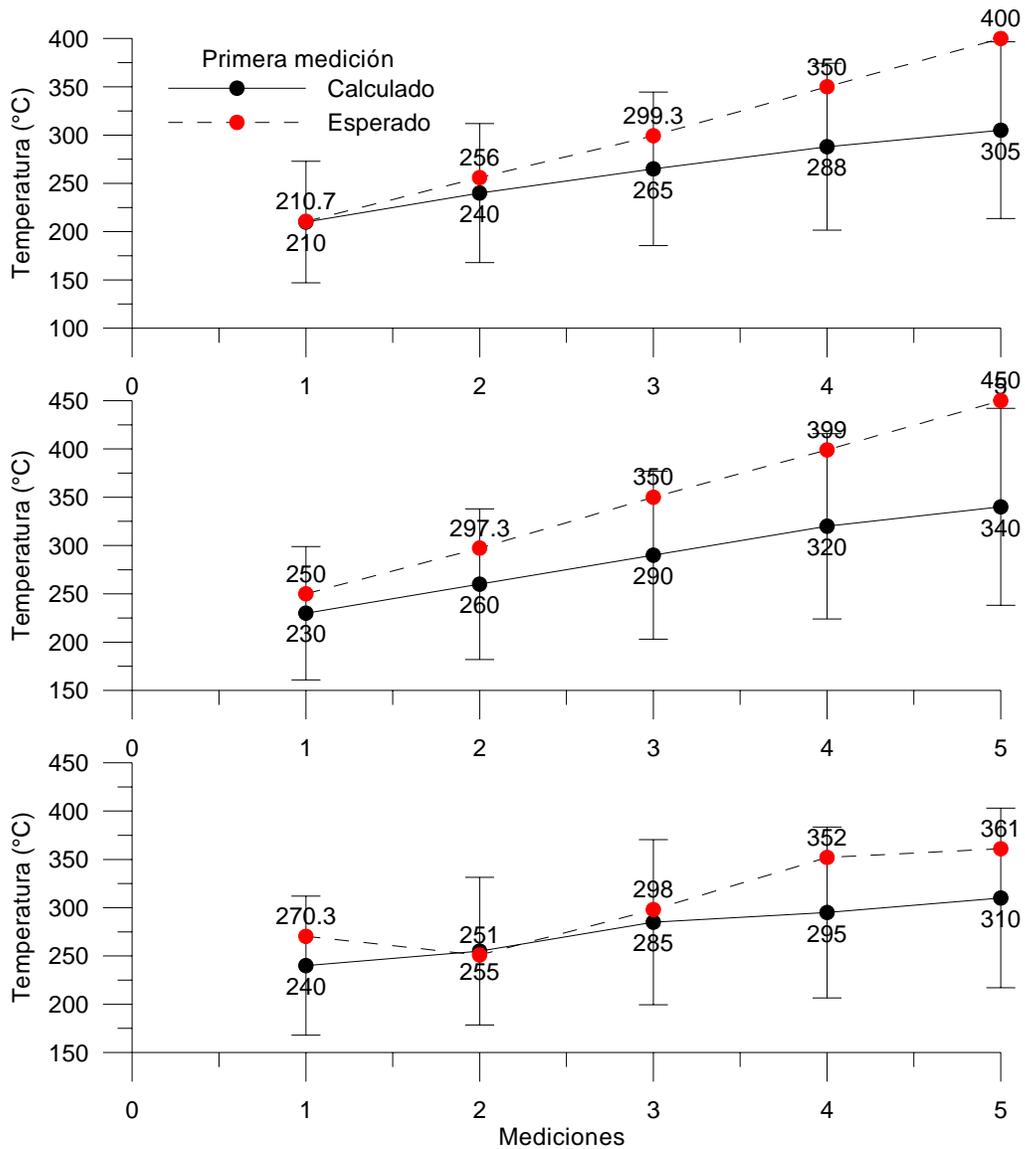


Figura 4.15 Esta figura muestra los resultados del cálculo de temperatura obtenido por MAPS en tres sesiones de medición. Las Barras de error en color rojo corresponden a la incertidumbre del sistema de control de temperatura estimado en 5% y las barras en color negro a la incertidumbre de MAPS para el cálculo de temperatura y concentraciones (30%).

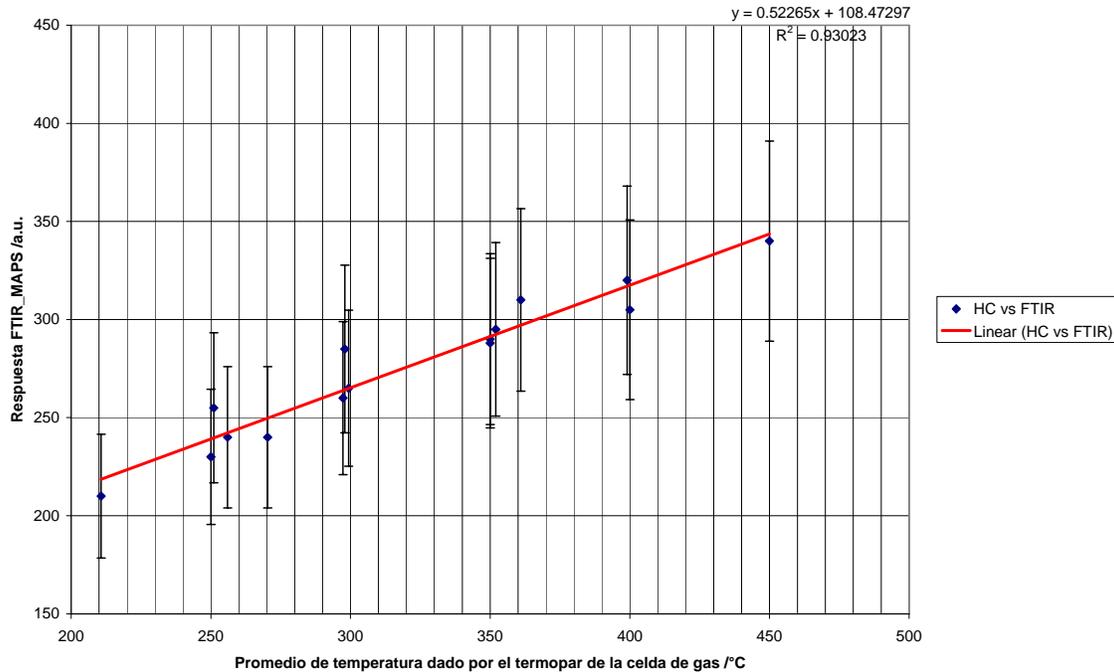


Figura 4.16 Respuesta en el calculo de temperatura del sistema de medición FTIR y software MALT con respecto al incremento de temperatura del gas contenido dentro de la celda de gas en el rango de 200-400°C. Las Barras de error en color negro corresponden a la incertidumbre del sistema FTIR y MAPS para el cálculo de temperatura y concentraciones (30%).

Una de las razones que pudieron influir el aumento de la discrepancia entre los valores de temperatura calculada por FTIR y reportada por los indicadores de la celda de gas, puede ser debido a los efectos de no-homogeneidad térmica existente dentro de la celda de gas. Sin embargo, debido a que puede ser asumida una respuesta lineal del sistema de medición FTIR con respecto a la lectura de temperatura de la celda de gas esta puede ser conocida utilizando simplemente la ecuación de respuesta dada en la figura 4.16.

Con el objetivo de estudiar el origen de la diferencia de temperatura dada por ambos sistemas, se realizaron mediciones del perfil de temperatura interna de la

celda de gas. La figura 4.17 muestra un esquema de estas mediciones en donde TA es la temperatura indicada por el termopar en posición A, TB en B y C en TC. Como resultado fue observado que cuando la celda de gas es sometida a temperaturas cercanas a los 400°C, coexisten zonas en la cuales la temperatura es cercana a los 400°C y zonas en las cuales esta es 120°C inferior manifestándose así el grado de inhomogeneidad de temperatura dentro de la celda de gas a altas temperaturas lo cual permite que gas presente en zonas frías absorba la radiación emitida por zonas de gas calientes produciéndose así efectos adversos para la cuantificación de temperatura del gas dentro de la celda. Resultados tabla 4.1.

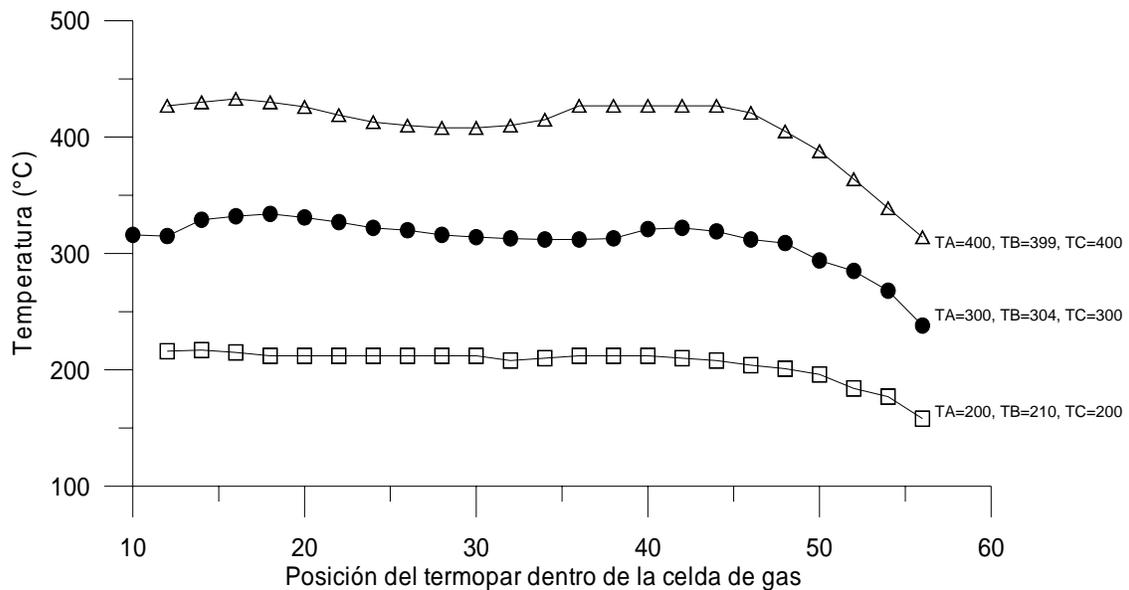


Figura 4.17 Perfil de temperatura dentro de la celda de gas a temperaturas de 205, 311 y 408°C medido por un termopar instalado en distintas posiciones dentro de la celda de gas. El promedio de temperatura en las distintas posiciones del gráfico resultó ser de 205, 311 y 408 para cada una de las temperaturas reportadas.

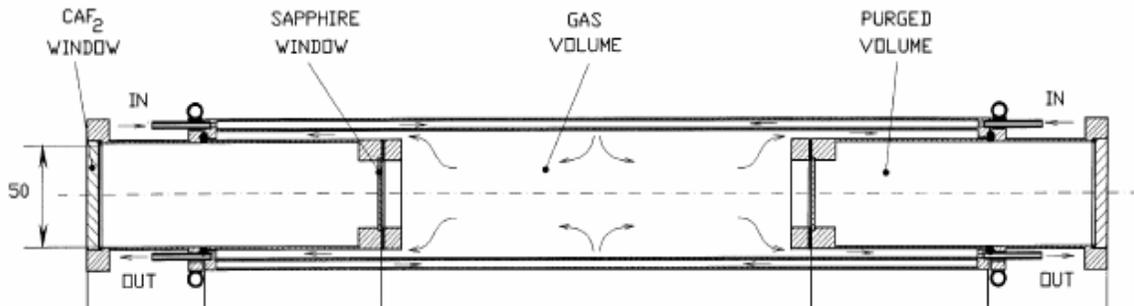
Tabla 4.1. Lectura de temperatura de un termopar introducido a la celda de gas a tres niveles de temperatura.

<i>Posición del termopar cm</i>	<i>Temperatura medida por el termopar de prueba (°C) Celda temperatura 1</i>	<i>Temperatura medida por el termopar de prueba (°C) Celda temperatura 2</i>	<i>Temperatura medida por el termopar de prueba (°C) Celda temperatura 3</i>
55	158	268	314
54	177	238	339
52	184	285	364
50	196	294	388
48	201	309	405
46	204	312	421
44	208	319	427
42	210	322	427
40	212	321	427
38	212	313	427
36	212	312	427
34	210	312	415
32	208	313	410
30	212	314	408
28	212	316	408
26	212	320	410
24	212	322	413
22	212	327	419
20	212	331	426
18	212	334	430
16	215	332	433
14	217	329	430
12	216	315	427
10	-	316	-
	<i>TA=200</i>	<i>TA=300</i>	<i>TA=400</i>
	<i>TB=210</i>	<i>TB=304</i>	<i>TB=399</i>
	<i>TC=200</i>	<i>TC=300</i>	<i>TC=400</i>
	<i>Temp Promedio=203</i>	<i>Temp Promedio=301</i>	<i>Temp Promedio=399</i>

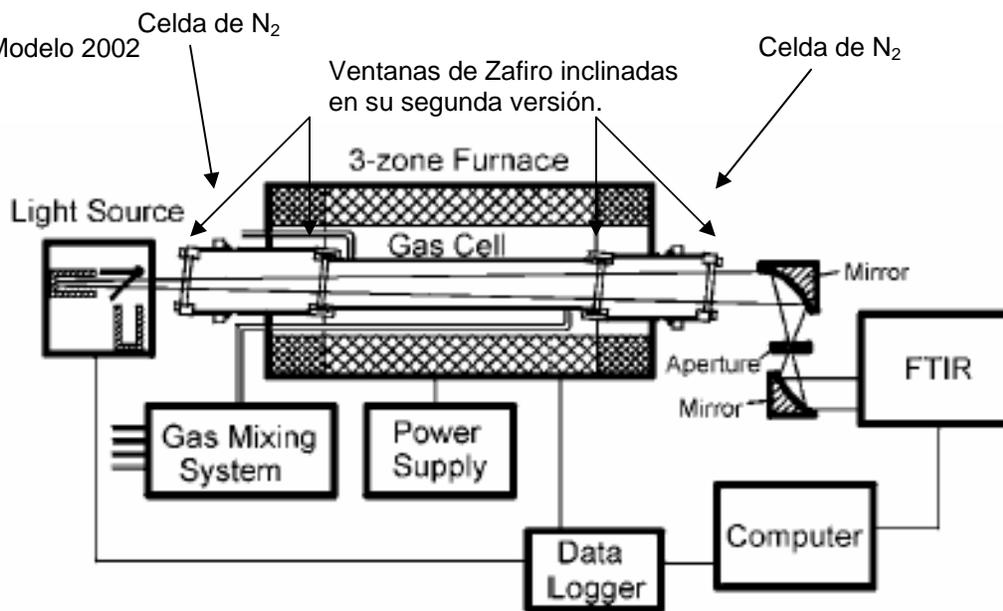
De esta investigación pudo concluirse que la celda de gas es un sistema estable para la medición de gases, sin embargo, resulta indispensable efectuar mejoras en su equipamiento técnico. Durante los últimos años S. Clausen et al. (1996 y 2002) han trabajado en la optimización de este tipo de celdas de gas, obteniendo como resultado un equipo capaz de elevar la temperatura interior de

la celda de gas hasta ~ 1100 K con homogeneidad en la distribución de temperatura dentro de la celda de gas de 2.3%. Entre las mejoras más importantes por Clausen. et al. (2002) se encuentra la inclusión en el sistema de la celda de gas de dos pequeñas mini-celdas de nitrógeno. Esta adecuación permite que la radiación recién emitida por los gases de calibración a alta temperatura no sufra absorciones durante su paso a la ventana frontal del espectrómetro. Así mismo, fueron incluidas ventanas inclinadas para reducir la reflexión y por tanto franjas de interferencia en el espectro medido. Así mismo, el sistema de calentamiento de la celda de gas de Clausen et al, permite elevar la temperatura de las paredes internas de la celda de gas a más de 1100 K con diferencias de temperatura del orden de ~ 25 K, por lo que es un sistema ideal para realizar comparaciones con alta calidad de resultados.

Clausen, Modelo 1997



Clausen, Modelo 2002



Auxitrol, m

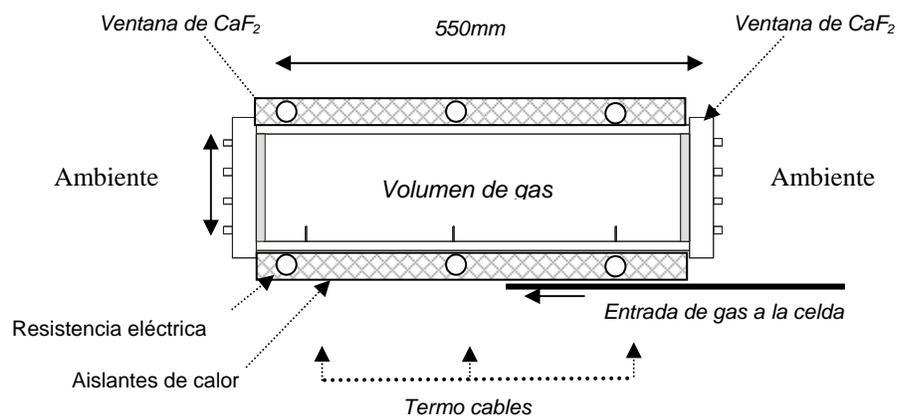


Figura 4.17. Sección transversal de tres modelos de celda de gas. a) Claussen et al., 1997, b) Claussen et al., 2002 y c) celda Auxitrol (utilizada en esta contribución).

CAPÍTULO

5

MEDICIÓN EN AEROPUERTOS DE AERONAVES EN OPERACIÓN

Llevar a cabo mediciones de gases de combustión producidos por motores de aeronaves es un área en donde la actual tecnología se reduce a estudios controlados en camas de pruebas de motores debido a las complicaciones técnicas que esta metodología requiere.

El contar con una técnica que permita la identificación y cuantificación de compuestos emitidos por aeronaves con una técnica de percepción remota, puede proveer de información tan importante como el conocimiento de los niveles de emisión de NO y CO en las diferentes etapas de operación del motor de una aeronave bajo condiciones reales de operación (Aeropuertos) y llevar a cabo estudios de las emisiones con respecto al envejecimiento de flota.

Durante la última década, se han podido realizar estudios de aeronaves mediante esta técnica bajo condiciones semi-controladas en distintos aeropuertos y camas de prueba de motores con una amplia cooperación de aerolíneas facilitando algunas de sus aeronaves y de los cuales se obtuvieron

resultados muy satisfactorios (detalles Heland et al., 1997y 1998, Schäfer et al., 2000 y 2003).

En esta contribución se buscó mejorar dichas mediciones al poderlas realizar en condiciones normales de operación, sin ninguna clase de asistencia de de las aerolíneas estudiadas. En el siguiente capítulo se muestra la evolución de las mediciones a lo largo de una campaña piloto en el aeropuerto internacional de la ciudad de Budapest y de una segunda campaña de medición realizada en el aeropuerto internacional de la ciudad de Zurich, ambas llevadas a cabo en el año 2004.

5.1 Instrumentación

Medir la radiación infrarroja para realizar el cálculo de concentración de los gases generados por aeronaves en condiciones normales de operación terrestres de las aeronaves requiere de instrumentación especializada. Esta afirmación está fundada en la dificultad operativa que exige la empresa de coleccionar radiación infrarroja emitida por una pluma de gas en constante movimiento y localizada a más de 40 metros de distancia. Por esta razón, el sistema de visualización de gases en el infrarrojo, descrita en el capítulo 3, resulta idóneo para dicha tarea. Las características técnicas ofrecidas por dicho sistema, como la localización de una fuente de gases a alta temperatura, el fácil manejo del campo de visión, las diferentes velocidades de colección de muestra,

la ligereza y practicidad de su instrumentación (menos de 23 kg), etc., hacen de este quipo de percepción remota el equipo adecuado para llevar a cabo dichos estudios.

5.2 Arreglo experimental

La obtención de los índices de emisión de las aeronaves fue realizada en dos etapas. La primera etapa consistió en la medición de la pluma de gas emitida por la Unidad de Poder Auxiliar (APU), llevada a cabo durante el estadio de la aeronave en la plataforma de abordaje (que usualmente tiene un lapso de 10 minutos). La segunda etapa consistió en la medición de los índices de emisión de la pluma de gas emitida por los turborreactores principales realizado durante el intervalo de tiempo intermedio entre dos operaciones de rutina, el remolque (momento en el que la aeronave es remolcada fuera de la plataforma de abordaje) y el desprendimiento (momento en el que el equipo de remolque es retirado del avión y la aeronave se próxima a partir), en el cual se cuenta con menos de 1 minuto para visualizar la fuente de radiación y realizar la medición de espectros a alta resolución. La siguiente secuencia de imágenes (figuras 5.1, 5.2 y 5.3) ejemplifica el procedimiento FTS y la obtención de espectros a alta resolución realizada durante operaciones de rutina de remolque y desprendimiento.

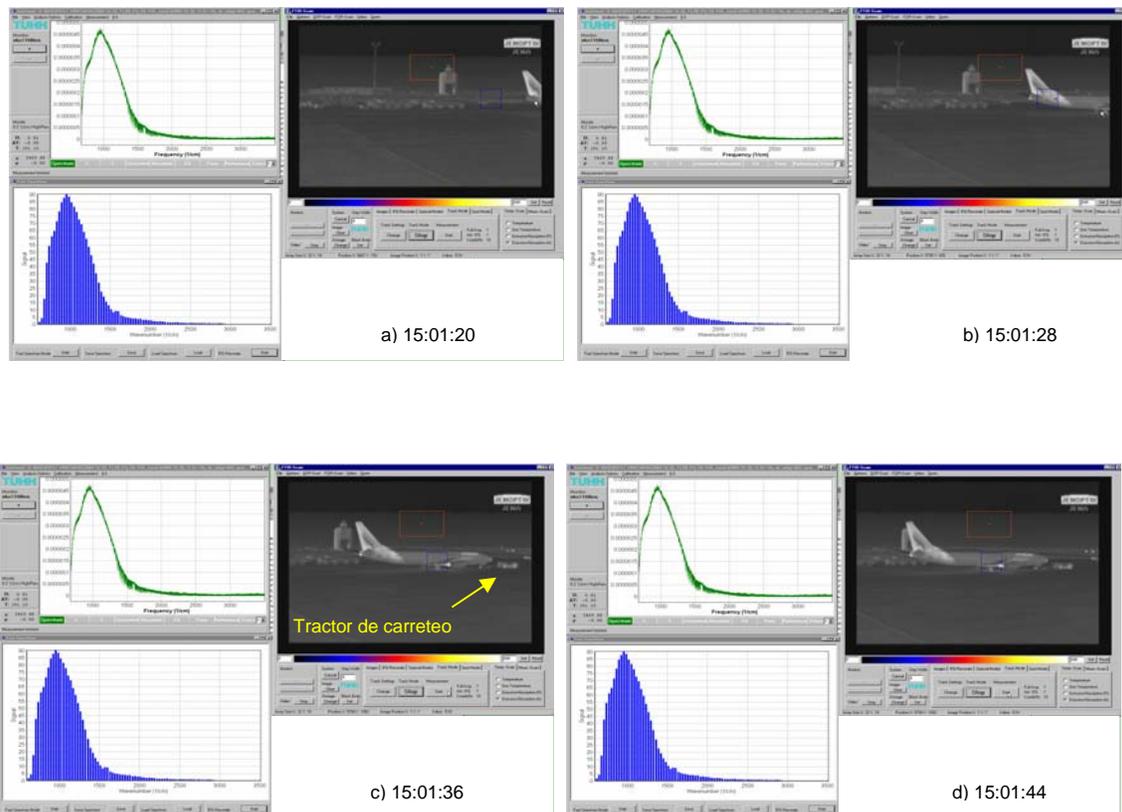


Figura 5.1. Secuencia de visualización (a-d) de la interfase del software GeDetekt del sistema SIGIS durante el remolque de una aeronave previa al carreteo en el aeropuerto internacional de la ciudad de Budapest en un lapso de 24 segundos. En esta imagen pueden apreciarse los tres principales módulos del software así como la actividad de uno solo de los tres módulos del software (el modulo de visualización por imágenes infrarrojas).

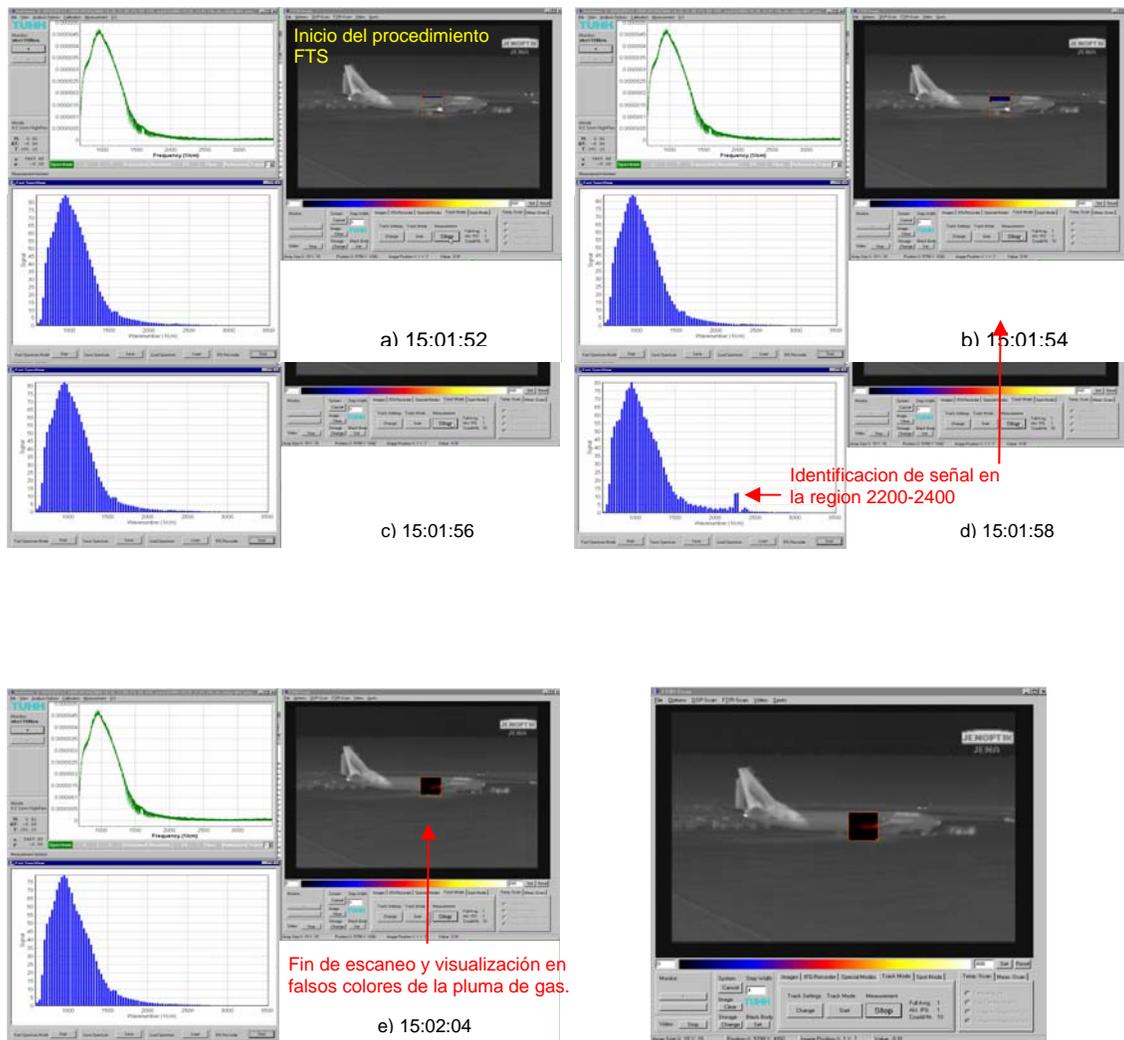


Figura 5.2. Secuencia de visualización de la interfase del software GeDetekt posterior al remolque, justo al iniciar el procedimiento FTS de la pluma de gases de escape el cual tomo en esta ocasión 12 segundos. Nótese el inicio del escaneo en la secuencia a) y la finalización de este procedimiento (secuencia e) en donde puede observarse las forma de la pluma de gas formada en falsos colores.

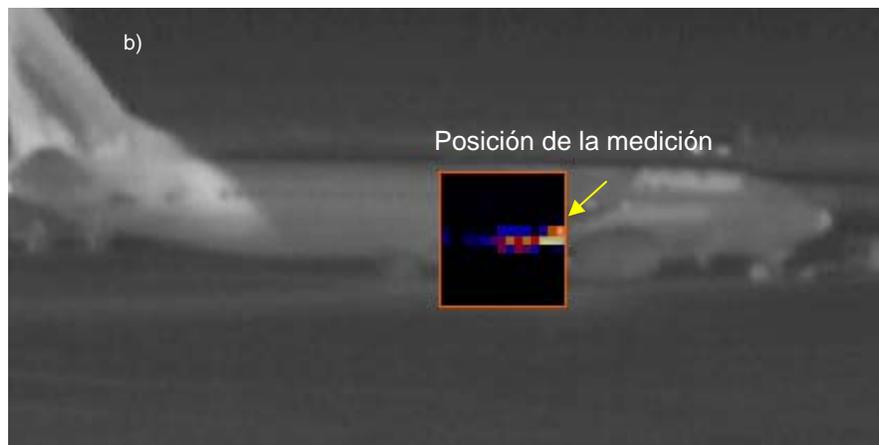
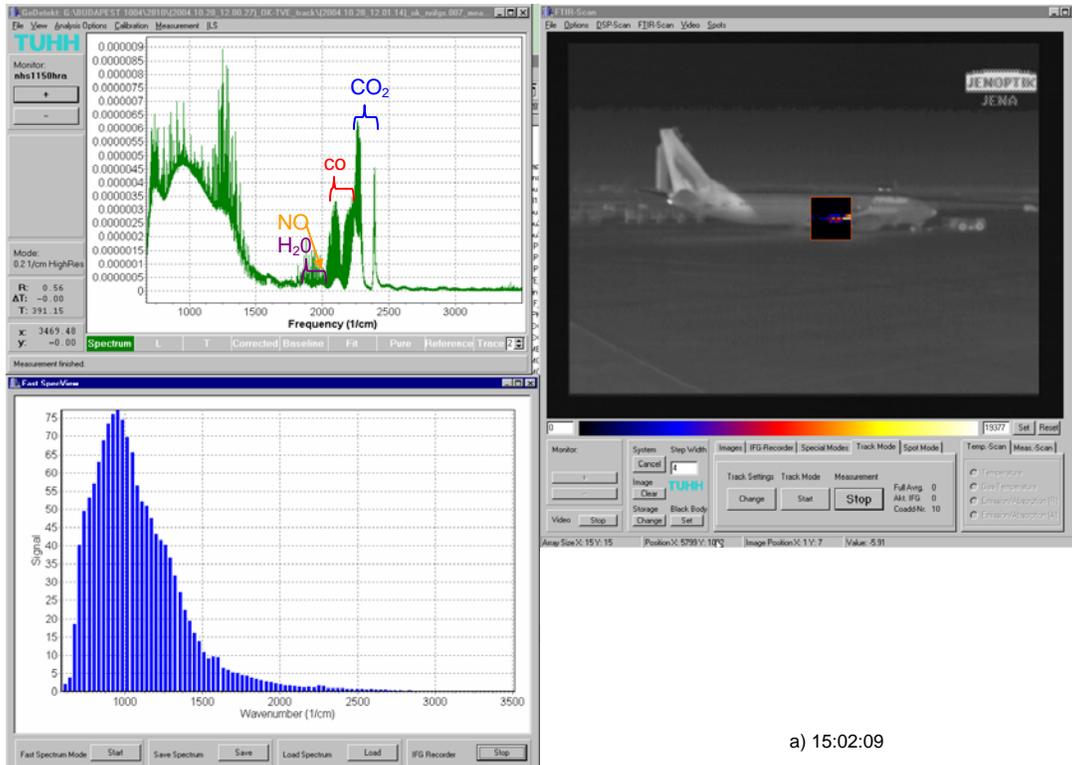


Figura 5.3. a) Visualización de la interfase del software GeDetekt durante la de espectros a alta resolución. b) Ampliación de la imagen proveniente de la ventana superior derecha que muestra la imagen infrarroja captada por el sistema SIGIS con falsos colores sobrepuestos resultado del procedimiento FTS.

5.3 Mediciones en el Aeropuerto Internacional de Zurich, Suiza.

En el mes de Julio del año 2004 se llevó a cabo una campaña de medición en el aeropuerto internacional de la ciudad de Zurich con el propósito de validar el modelo de dispersión de contaminantes de este aeropuerto é iniciar mediciones piloto con el sistema SIGIS. Durante la campaña de medición, se probaron diferentes versiones del software de adquisición de espectros GeDetekt modificado de su versión original para esta nueva aplicación, así como la actualización del software MAPS para la interpretación de los espectros a alta resolución. De esta forma los objetivos generales de la primera campaña de medición del sistema SIGIS fueron:

- Identificar posibles problemas técnicos y requerimientos adicionales para efectuar mediciones en campo por el sistema SIGIS,
- probar la eficacia del procedimiento FTS para la visualización de una fuente de emisión de radiación infrarroja (una pluma de gas caliente) localizada a más de 40 metros de distancia,
- obtener los primeros espectros a alta resolución emitidos por una turbina ubicada a una distancia no menor a 40 metros y
- efectuar la determinación de la concentración de gases a través de la actualización del software MAPS.

El lugar de instalación del sistema SIGIS fue designado entre dos plataformas de abordaje (A48 y A49) pues en este sitio el campo de visión fue muy privilegiado

y no existió ninguna clase de inconveniente con las normas de seguridad del aeropuerto. La figura 5.4 muestra el lugar de instalación y los campos de visión para la medición de los espectros.



Figura 5.4 a) Imagen en donde se muestra la posición de medición del sistema SIGIS para los motores de las aeronaves. b) sistema SIGIS durante la medición c) Campo de visión para la medición de las emisiones del APU durante la estadia de las aeronaves en plataforma.

5.3.1 Mediciones y resultados

A continuación se enlistan las mediciones realizadas durante esta campaña piloto de medición:

Procedimiento FTS:

- Airbus A321-111 (Swiss International Air Lines) número de identificación HB-IOC,
- Boeing 767-224(ER) (Continental Airlines) número de identificación N76151,
- Airbus A330-223 (Swiss International Air Lines) número de identificación HB-IQP,
- Airbus A330-223 (Swissair) número de identificación HB-IQA,
- Airbus A319-112 (Swiss International Air Lines) número de identificación HB-IPV.

Medición de espectros a alta resolución:

- Avro RJ85 (British Aerospace) número de identificación HB-IYY,
- Airbus A319-112 (Swiss International Air Lines) número de identificación HB-IPR,
- Avro RJ100 (British Aerospace) número de identificación HB-IYX,

- Airbus A319-112 (Swiss International Air Lines) número de identificación HB-IPV,
- Boeing 767-224 (ER) (Continental Airlines) número de identificación N68155,
- McDonnell Douglas MD-11 (Swiss International Air Lines) número de identificación HB-IWE,
- Boeing 767-224(ER) (Continental Airlines) número de identificación N69154,
- Airbus A340-313X (Swiss International Air Lines) número de identificación HB-JMF,
- Airbus A330-223 (Swiss International Air Lines) número de identificación HB-IQP.

La imagen 5.6 muestra el resultado de la aplicación del procedimiento FTS en el que fue analizado el escape del APU de una aeronave Airbus A321-111 ubicada a una distancia de 37 metros del sistema SIGIS. En la secuencia de imágenes pueden observarse zonas del motor relativamente más calientes (figura 5.6a) así como el resultado del procedimiento FTS en las regiones 772 a 1203 cm^{-1} (figura 5.6b) 2191 a 2314 cm^{-1} (figura 4.69c) y 2345 a 2406 cm^{-1} (figura 5.6d) con el objetivo de localizar dentro del campo de visión la estructura del motor, la pluma de gas y de las zonas de mayor contenido de CO_2 , respectivamente.

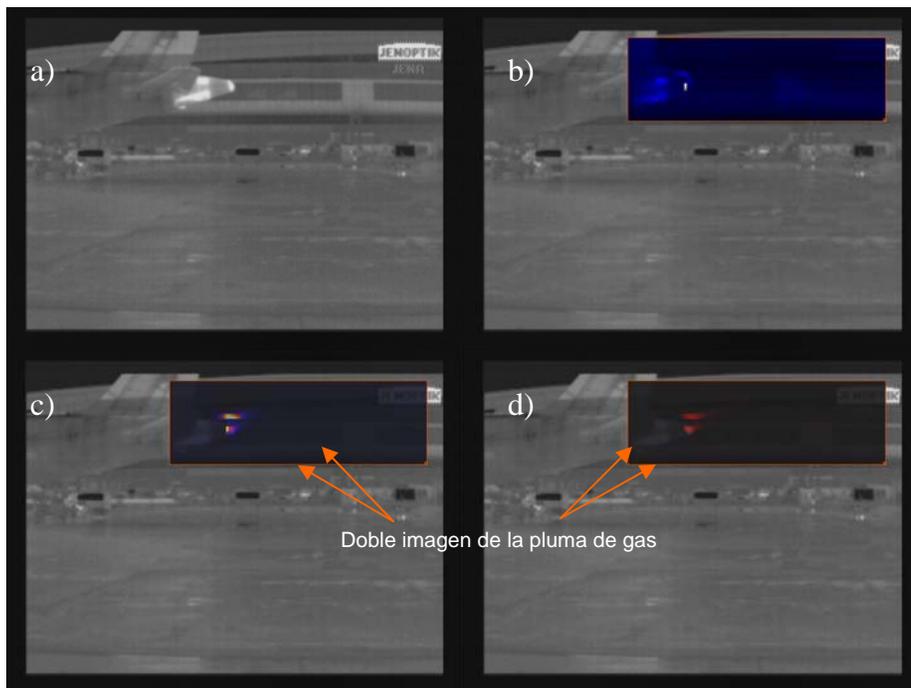


Figura 5.6. Secuencias de imágenes infrarrojas sobrepuestas por falsos colores resultado del procedimiento FTS del APU de la aeronave Airbus A321-111 resultado del análisis de las regiones 772-1203 (b), 2191-2314 (c) y 2345-2406 cm^{-1} (d).

La figura 5.7 muestra de igual forma el procedimiento FTS aplicado al motor principal del Airbus A321-111, localizado a una distancia de 40 metros. Al igual que en la imagen anterior, en ésta imagen pueden observarse dos plumas de gas debido al desalineamiento óptico del espectrómetro durante esta campaña de medición.

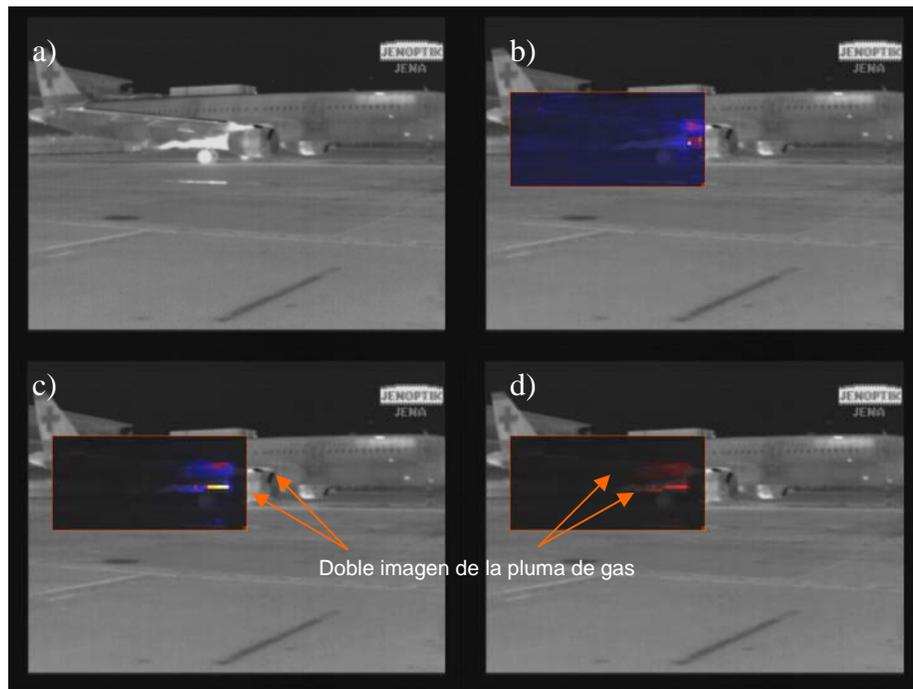


Figura 5.7. Secuencias de imágenes infrarrojas sobrepuestas por falsos colores resultado del procedimiento FTS al del motor tipo CFM56-5B1/2 de la aeronave Airbus A321-111 resultado del análisis de las regiones 772-1203 (b), 2191-2314 (c) y 2345-2406 cm^{-1} (d).

Las figuras (5.8, 5.9, 5.10 y 5.11) muestran el mismo procedimiento aplicado a las aeronaves Boeing 767-224(ER) (N76151), Airbus A330-223 (HB-IQP), Airbus A330-223 (HB-IQA) y Airbus A319-112 (HB-IPV).

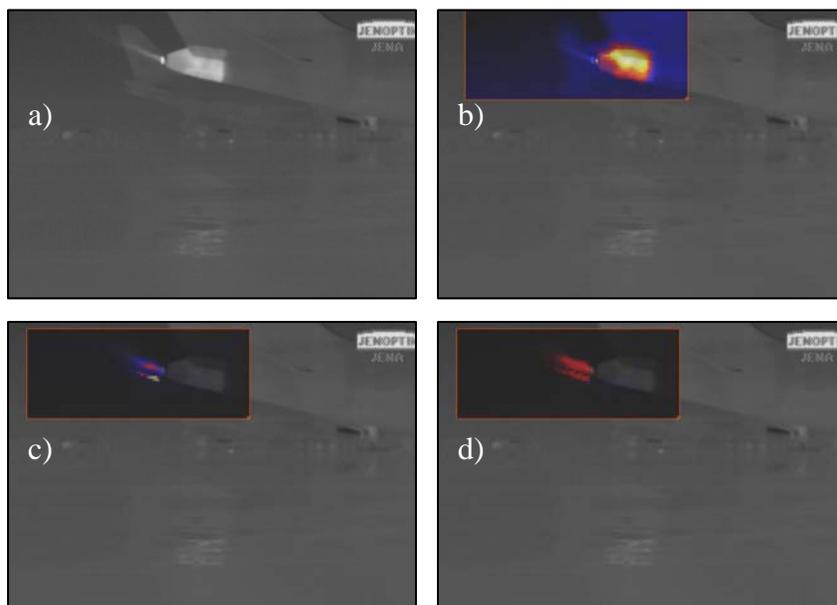


Figura 5.8. Secuencias de imágenes infrarrojas sobrepuestas por falsos colores resultado del procedimiento FTS del APU de la aeronave Boeing 767-224(N76151) resultado del análisis de las regiones 772-1203 (b), 2191-2314 (c) y 2345-2406 cm^{-1} (d).

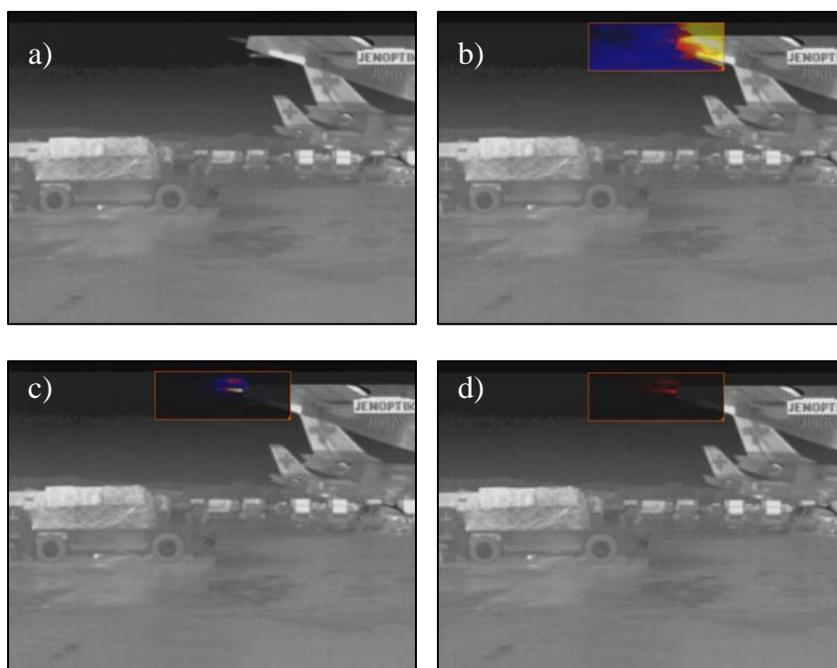


Figura 5.9. Secuencias de imágenes infrarrojas sobrepuestas por falsos colores resultado del procedimiento FTS del APU de la aeronave Airbus A330-223 (HB-IQP) resultado del análisis de las regiones 772-1203 (b), 2191-2314 (c) y 2345-2406 cm^{-1} (d).

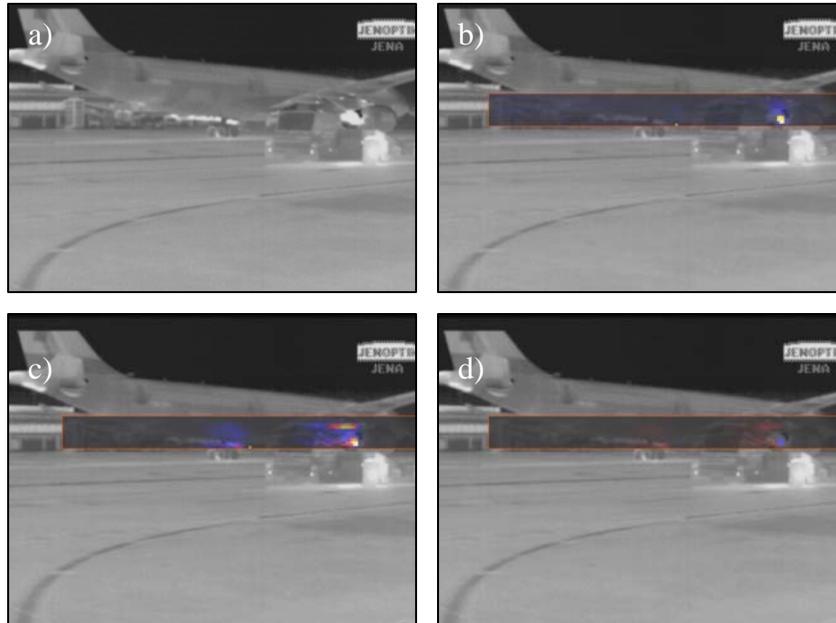


Figura 5.10. Secuencias de imágenes infrarrojas sobrepuestas por falsos colores resultado del procedimiento FTS del APU de la aeronave Airbus A330-223 (HB-IQA) resultado del análisis de las regiones 772-1203 (b), 2191-2314 (c) y 2345-2406 cm^{-1} (d).

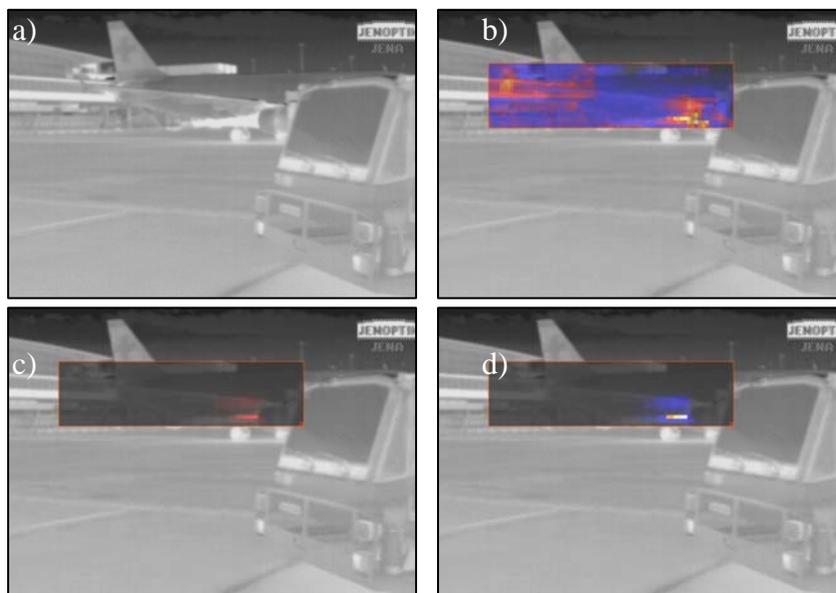
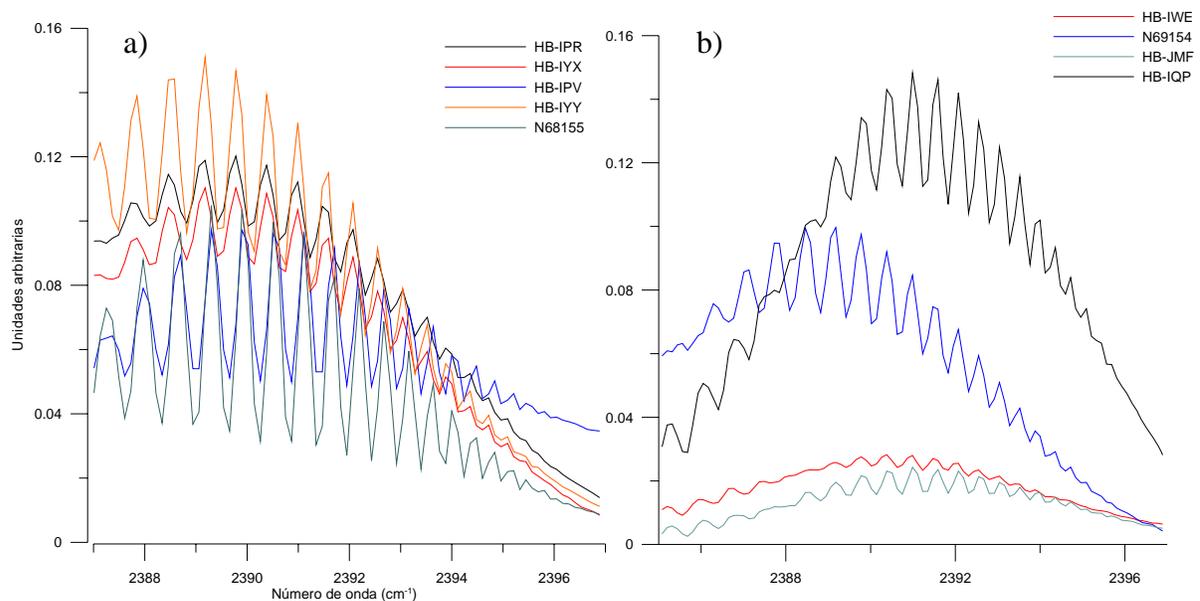


Figura 5.11. Secuencias de imágenes infrarrojas sobrepuestas por falsos colores resultado del procedimiento FTS del APU de la aeronave Airbus A319-112 (HB-IPV) resultado del análisis de las regiones 772-1203 (b), 2191-2314 (c) y 2345-2406 cm^{-1} (d).

En la segunda etapa experimental se obtuvieron espectros de emisión a alta resolución de nueve aeronaves (figuras 5.12 a y b) sin embargo, debido al desalineamiento del instrumento sólo los espectros de emisión de las aeronaves Avro RJ85 (HB-IYY) y Boeing 767-224 (N68155), pudieron ser interpretados.



5.12 Espectros infrarrojos de emisión no calibrados obtenidos de los gases de combustión de las aeronaves a) Avro RJ85 número de identificación HB-IYY, Airbus A319-112 número de identificación HB-IPR, Avro RJ100 número de identificación HB-IYX, Airbus A319-112 número de identificación HB-IPV, Boeing 767-224(ER) número de identificación N68155 y b) McDonnell Douglas MD-11 número de identificación HB-IWE, Boeing 767-224(ER) número de identificación (N69154), Airbus A340-313X número de identificación HB-JMF), Airbus A330-223 número de identificación HB-IQP.

Las figuras 5.13 (a y b) muestran las termo imágenes de la aeronave Avro RJ85 (HB-IYY) captadas al momento de la medición de los espectros. El cálculo de temperatura de la pluma de gas emitida por el APU y la turbina de la aeronave Avro RJ85 dio como resultado $270\pm 81^{\circ}\text{C}$ y $280\pm 84^{\circ}\text{C}$ respectivamente, y de densidad de columna de $1.2\pm 0.3 \text{ E}+18$ y $5.0\pm 1.5 \text{ E}+18$ moléculas por cm^2 de CO.



Figura 5.13. a) Imagen infrarrojas antes del procedimiento FTS del APU tipo APS 3200. b) Imagen infrarrojas posterior al procedimiento FTS de medición del APU.

En el caso de la aeronave Boeing 767-224 de (figura 5.14) la densidad de columna calculada para CO₂, CO H₂O del APU fue de 2.94±0.88 E+18, 5.88±1.76 E+18 y 3.50±1.05 E+18 moléculas por cm² respectivamente.

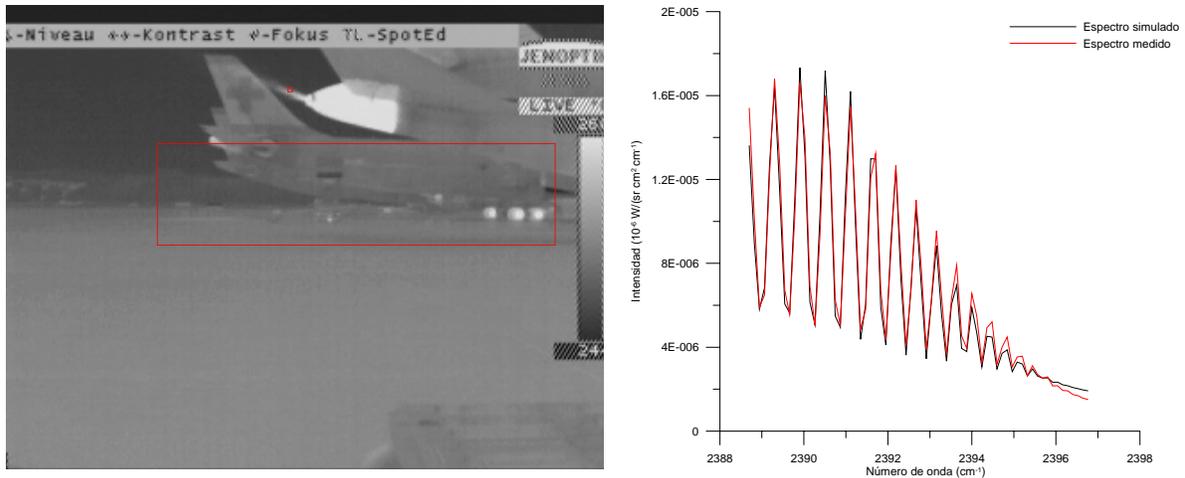


Figura 5.14. Izquierda: Imagen infrarroja del APU de la aeronave Boeing 767-224 en la cual puede observarse la posición en la que fue obtenido el espectro de emisión radiométricamente calibrados graficado en la posición derecha con su simulación del espectro producida por MAPS.

5.3.2 Conclusión

Durante esta campaña de medición se identificaron múltiples problemas técnicos del sistema SIGIS, entre los que se identificaron como los más graves; el fallo general del sistema produciendo la pérdida de mediciones, la falta de comunicación entre los puertos de video y el más importante, la desalineación de la óptica del espectrómetro responsable de un efecto de visualización de imágenes de plumas de gas dobles ,así como de la baja resolución observada en la mayoría de los espectros de emisión obtenidos.

A pesar de estos problemas técnicos, fue posible verificar la eficacia del procedimiento FTS, para la visualización de fuentes de emisión de radiación infrarroja, tras la obtención de espectros a alta resolución en posiciones ubicadas a 40 metros de distancia efectuándose la determinación de concentración de dos aeronaves a través del software MAPS actualizado con la inclusión de la función ILS del espectrómetro OPAG 22.

5.4 Aeropuerto Internacional de Budapest, Hungría.

El sistema SIGIS fue utilizado nuevamente durante la campaña de medición del aeropuerto internacional de la ciudad de Budapest Hungría en octubre de 2004, con el objetivo de visualizar fuentes de emisión de radiación infrarroja a través del procedimiento FTS para obtener espectros de emisión a alta resolución y efectuar la determinación de la concentración de compuestos producidos por las aeronaves.

El sistema SIGIS fue nuevamente ubicado entre dos plataformas de acenso de pasajeros, sin embargo, en esta ocasión el lugar resultó altamente inconveniente para efectuar mediciones debido a obstáculos no previstos en el campo de visión (autobuses-cabina estacionados frente a nuestros instrumentos) por lo que se optó por el uso de una escalinata con el fin de obtener un punto de visión superior a los obstáculos (Figura 5.15).

5.4.1 Mediciones y resultados

A continuación se enlistan las aeronaves medidas durante esta campaña de medición. La realineación de la óptica interna del espectrómetro y la mejora del software de adquisición de espectros GeDetekt, nos permitió en esta ocasión, la obtención de un mayor número de espectros de mejor calidad.

- McDonnell Douglas MD-11(F) (Varig Log) número de identificación HA-LOG,
- Boeing 737-86Q (Travel Service) número de identificación OK-TVE,
- Airbus A320-211 (Tunisair) número de identificación TS-IMF,
- Fokker 100 (Air Berlin) número de identificación D-AGPK,
- Boeing 737-3Y0 (Malév Hungarian Airlines) número de identificación HA-LEX,
- Fokker 70 (Malév Hungarian Airlines) número de identificación HA-LMB,
- Fokker 70 (Malév Hungarian Airlines) número de identificación HA-LMC,
- Boeing 737-8Q8 (Malév Hungarian Airlines) número de identificación HA-LOM.



Figura 5.15 a) Escalera utilizada durante las mediciones en el aeropuerto internacional de la ciudad de Budapest Hungría. b) Nuevo campo de visión del instrumento sobre la escalera. c) Imagen durante la medición.



Figura 5.16 Termo imágenes capturadas durante la medición de espectros a alta resolución de las aeronaves McDonnell Douglas MD-11 (HA-LOG), Boeing 737-7Q8 (HA-LOP), Boeing 737-86Q (OK-TVE), Airbus A320-211 (TS-IMF), Fokker 100 (D-AGPK), Boeing 737-3Y0 (HA-LEX), Fokker 70 (HA-LMB), Fokker 70 (HA-LMC), Boeing 737-8Q8 (HA-LOM).

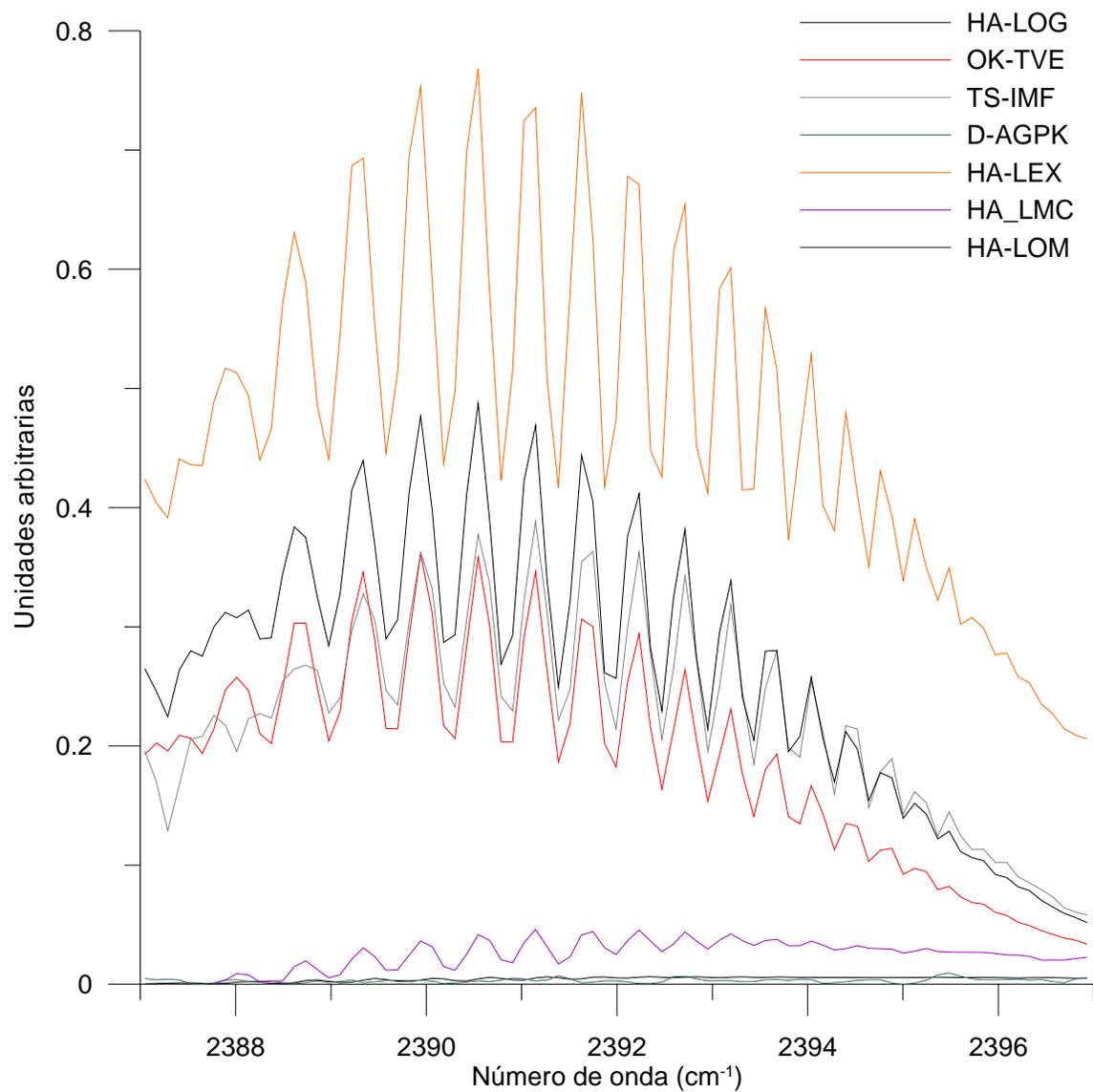


Figura 5.17 Espectros infrarrojos de emisión no calibrados medidos de los gases de emisión de las aeronaves McDonnell Douglas MD-11(F) con el número de identificación HA-LOG, Boeing 737-86Q con el número de identificación OK-TVE, Airbus A320-211 con el número de identificación TS-IMF, Fokker 100 con el número de identificación D-AGPK, Boeing 737-3Y0 con el número de identificación HA-LEX, Fokker 70 con el número de identificación HA-LMB, Fokker 70 con el número de identificación HA-LMC, Boeing 737-8Q8 con el número de identificación HA-LOM.

La tabla 5.1 y la figura 5.18 muestran los resultados cuantitativos de los espectros de emisión de cuatro aeronaves (números de identificación TS-IMF, HA-LEX, OK-TVE y HA-LOM) medidas a 120, 80 y 100 metros de distancia respectivamente. Las aeronaves TS-IMF y HA-LOM fueron medidas en más de una ocasión debido al retraso en su salida lo cual permitió efectuar mediciones por períodos de tiempo más prolongados. Los resultados de temperatura calculado por MAPS variaron de 300 á 465 °C y la densidad de columna de CO fue estimada de entre 1.25E+17 a 4.33E+17 moléculas por cm³ en el caso de las aeronaves locales (HA-LOM) ~>60% superior. En el grafico de la figura 5.18 puede notarse que el nivel de concertación de CO emitido por las aeronaves en donde destacan las aeronaves locales por su alta emisión.

Identificación de la Aeronave	Temperatura (°C)	CO ₂ (moléculas por cm ²)	CO (moléculas por cm ²)	H ₂ O (moléculas por cm ²)
HA-LEX	465 ± 139	9.04 ± 2.71E+18	1.25 ± 0.38E+17	1.14 ± 0.34E+19
OK-TVE	300 ± 90	3.90 ± 1.17E+19	2.62 ± 0.79E+17	3.37 ± 1.01E+19
TSIMF	320 ± 96	4.91 ± 1.48E+19	3.11 ± 0.93E+17	5.56 ± 1.67E+19
TS-IMF2	360 ± 108	1.48 ± 0.47E+19	1.81 ± 0.55E+17	2.26 ± 0.67E+19
HA-LOM	320 ± 96	4.70 ± 1.41E+19	4.33 ± 1.30E+17	3.71 ± 1.11E+19
HALOM2	350 ± 105	4.18 ± 1.25E+19	4.12 ± 1.20E+17	3.53 ± 1.05E+19
HALOM3	410 ± 123	4.31 ± 1.30E+19	3.08 ± 0.92E+16	3.22 ± 0.96E+19

Tabla 5.1. Resultados cuantitativos de los espectros medidos durante la campaña de medición del aeropuerto internacional de la ciudad de Budapest.

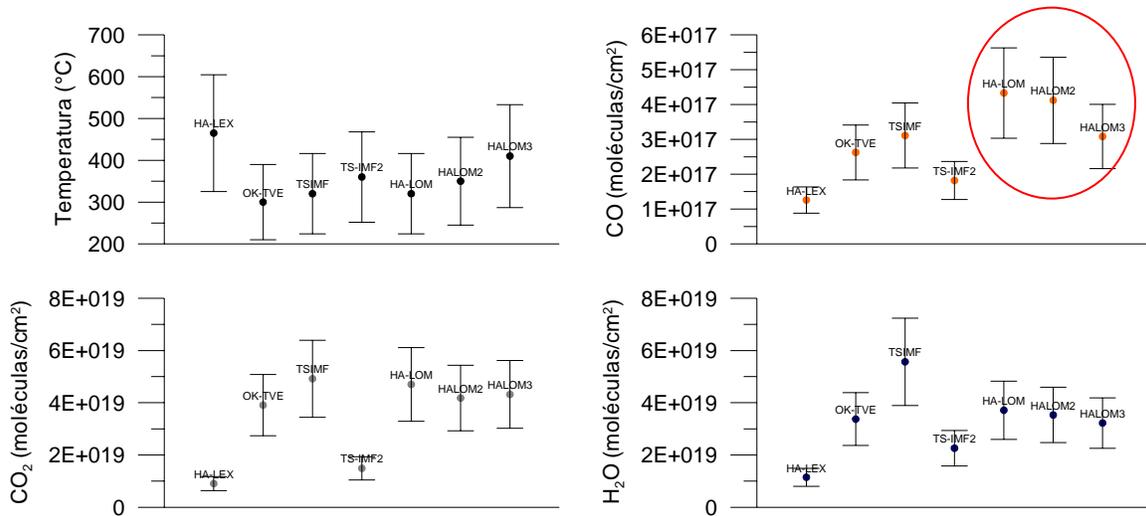


Figura 5.18 Resultados del análisis cuantitativo de los espectros colectados por el sistema SIGIS de las aeronaves McDonnell Douglas MD-11 (HA-LOG), Boeing 737-86Q (OK-TVE), Airbus A320-211 (TS-IMF), Fokker 100 (D-AGPK), Boeing 737-3Y0 (HA-LEX), Fokker 70 (HA-LMB), Fokker 70 (HA-LMC), Boeing 737-8Q8 (HA-LOM).

5.4.2 Conclusión

La alineación de la óptica del espectrómetro OPAG 22, el mejoramiento del software GeDetekt y la reparación de los puertos de video del sistema SIGIS permitieron el correcto funcionamiento del procedimiento FTS para la visualización y localización de las fuentes de emisión. A través este procedimiento se obtuvieron los espectros a alta resolución para la determinación de la temperatura así como de la concentración de CO, CO₂ y H₂O de cuatro aeronaves ubicadas a una distancia promedio de 100 metros de distancia. Con esto se pudo demostrar tanto la capacidad de medición del sistema SIGIS como la interpretación de resultados por el nuevo software MAPS.

CAPÍTULO

6

MEDICIÓN DE UN TURBOREACTOR EN UNA CAMA DE PRUEBAS

En el mes de septiembre del año 2005 se realizó una campaña de medición con el objetivo de caracterizar los gases de combustión generados por el turborreactor Gnome 1200, normalmente utilizado en la propulsión de helicópteros Westland Wessex, a través de dos equipos de percepción remota (sistema SIGIS y un espectrómetro del proyecto AEROTEST), así como un arreglo instrumental de mediciones in-situ. Desafortunadamente, debido a problemas de logística con el grupo encargado de las mediciones in-situ, solo las mediciones por percepción remota fueron realizadas. El sistema SIGIS fue utilizado con los objetivos de obtener espectros infrarrojos a alta resolución en configuración vertical y horizontal así como para identificar la distribución de temperatura y concentración de gases (NO y CO) en la corriente de gases.

6.1 Arreglo experimental

El turborreactor fue instalado dentro de la cama de pruebas a través de la remoción de la turbina de poder y el conducto, que gira al escape en 90 grados, reemplazado este último por un conducto de tubería jet, de tal manera que

finalmente el motor Gnome fue más parecido a un pequeño turboreactor con temperatura y velocidad superiores (figura 5.1 a, b y c). El sistema SIGIS, al igual que el espectrómetro del proyecto AEROTEST, fueron ubicados dos metros de distancia de la pluma de gas.



Figura 6.1. a) Helicóptero Westland Wessex b) Motor de propulsión Gnome 1200 desarrollado por la compañía Rolls-Royce c) Motor Gnome 1200 modificado para su instalación en una cama de pruebas d) Motor Gnome 1200 en operación.

6.2 Mediciones y resultados

En la primera etapa de mediciones, el procedimiento FTS y mediciones a alta resolución fueron realizadas con el sistema SIGIS con el objetivo de localizar posiciones óptimas de medición en la pluma de gas. Posteriormente, se colectaron espectros a alta resolución en diferentes secuencias (vertical y horizontal) a distintas velocidades de operación de la turbina. A continuación se enlista en forma detallada y secuencial el desarrollo de las mediciones en donde puede apreciarse el proceso de localización de posiciones hasta la obtención de los espectros a alta resolución.

- Calibración óptica del procedimiento FTS del sistema SIGIS utilizando un filtro óptico transparente a la región $900 \text{ a } 1000\text{cm}^{-1}$ (ver figura 6.2),
- Calibración fina óptica del procedimiento FTS del sistema SIGIS utilizando un filtro óptico transparente a la región $900 \text{ a } 1000\text{cm}^{-1}$ (ver figura 6.3),
- Medición de espectros a alta resolución en una posición con velocidad de operación del turborreactor de 20000 revoluciones por minuto (RPM) (figura 6.4),
- Medición de espectros a alta resolución en secuencia vertical con velocidad de operación del turborreactor fue de 20000 RPM (figura 6.5),
- Procedimiento FTS para la medición de espectros a alta resolución en una posición con velocidad de operación del turborreactor de 20000 RPM (figura 6.6),

- Procedimiento FTS para la medición de espectros a alta resolución en una posición con velocidad de operación del turborreactor de 20000 RPM (figura 6.7),
- Procedimiento FTS para la medición de espectros a alta resolución en una posición. La velocidad de operación del turborreactor decreció de 21000 RPM a 2000 RPM debido a un problema técnico (figura 6.8),
- Medición de espectros a alta resolución en secuencia vertical en 8 posiciones con velocidad de operación del turborreactor de 21500 RPM (figura 6.9),
- Medición de espectros a alta resolución en secuencia vertical (16 posiciones) con velocidad de operación del turborreactor de 19000 RPM. En los espectros de emisión pueden observarse importantes diferencias en intensidad y forma de línea de acuerdo a las distintas posiciones de escaneo (figura 6.10)
- Medición de espectros a alta resolución en secuencia vertical (16 posiciones) con velocidad de operación del turborreactor fue de 22500 RPM (figura 6.11),
- Medición de espectros a alta resolución en secuencia vertical (16 posiciones) con velocidad de operación del turborreactor fue de 20000 RPM (figura 6.12),
- Medición de espectros a alta resolución en secuencia vertical y horizontal (32 posiciones) con velocidad de operación del turborreactor fue de 20000 RPM (figura 6.13),
- FTS en secuencia vertical y horizontal con velocidad de operación de 20000 RPM (figura 6.14),
- Procedimiento FTS en el instante de efectuar interrupciones de combustible. La velocidad de operación del turborreactor vario de 20000 a 1000 RPM figura 6.15,

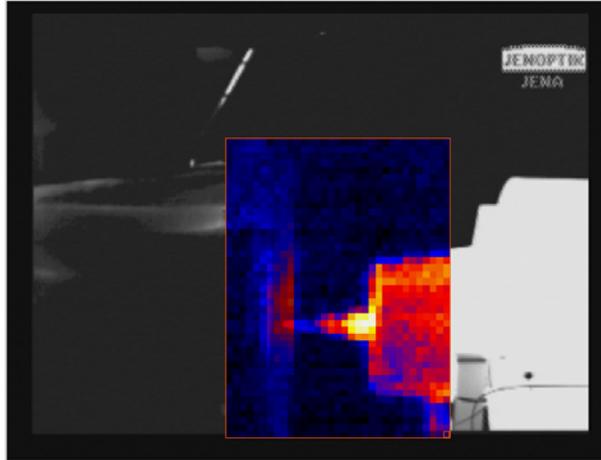


Figura 6.2. Termo-Imagen sobre puesta por falsos colores creada a través del proceso FTS programado para tomar espectros a baja resolución en secuencia vertical y horizontal utilizando un filtro óptico en la región $900-1000\text{cm}^{-1}$ y un ancho de paso del número 3 en el sistema SIGIS.

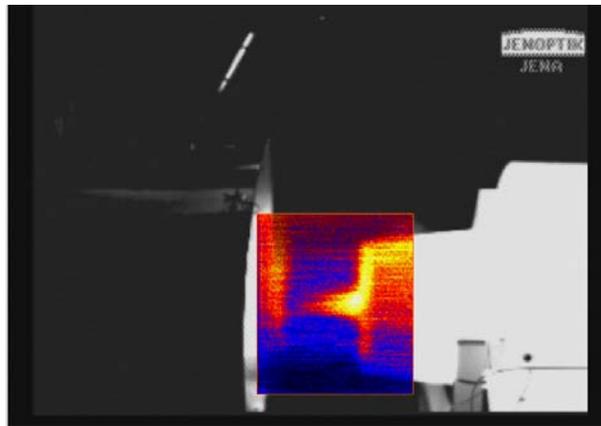


Figura 6.3. Termo-Imagen sobre puesta por falsos colores creada a través del proceso FTS programado para tomar espectros a baja resolución en secuencia vertical y horizontal utilizando un filtro óptico en la región $900-1000\text{cm}^{-1}$ y un ancho de paso del número 1 en el sistema SIGIS.

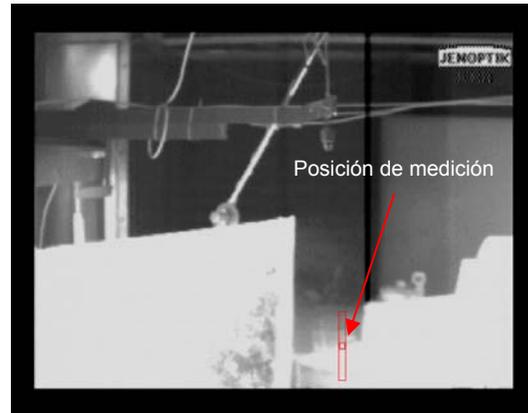
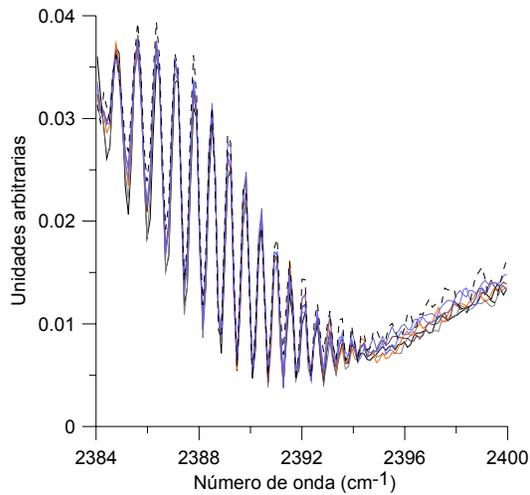


Figura 6.4. Espectros de emisión (izquierdo) y temo-imagen del escape del turborreactor RR (lado derecho) durante la medición de espectros a alta resolución en una posición en los que puede observarse la deformidad en los espectros de emisión de CO₂ debido a la posición de la obtención de los espectros pues ésta fue posada sobre parte de la superficie metálica del escape de la turbina. La velocidad de trabajo del turborreactor durante la medición fue de 20000 RPM.

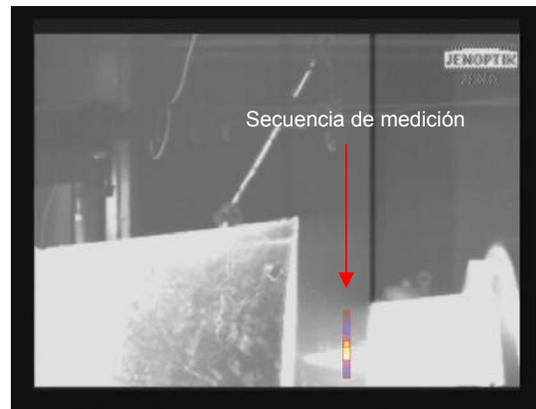
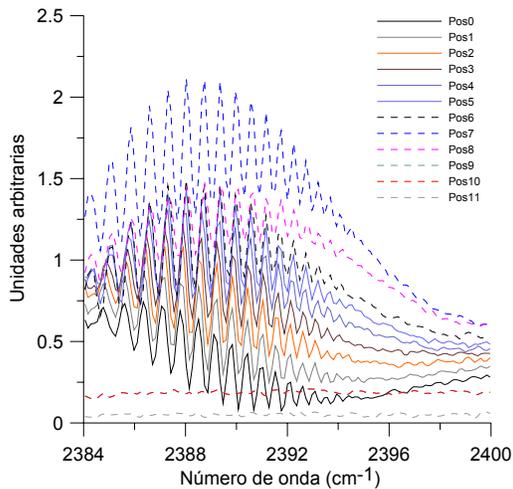


Figura 6.5. Espectros de emisión (izquierdo) y temo-imagen del escape del turborreactor RR (lado derecho) durante la medición de espectros a alta resolución en secuencia vertical. En los espectros puede observarse aun una extraña interferencia en los espectros de emisión de CO₂ colectados a través de las diferentes posiciones. La velocidad del turborreactor durante la medición fue de 20000 RPM.

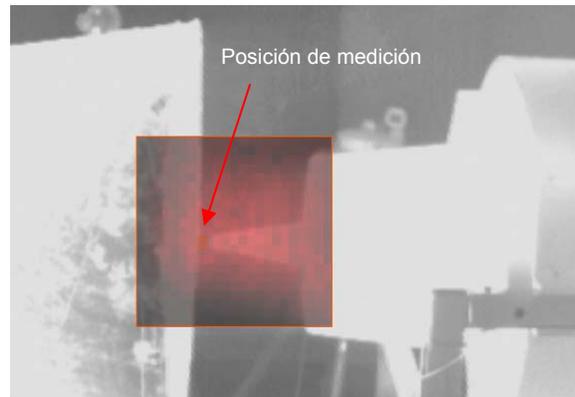
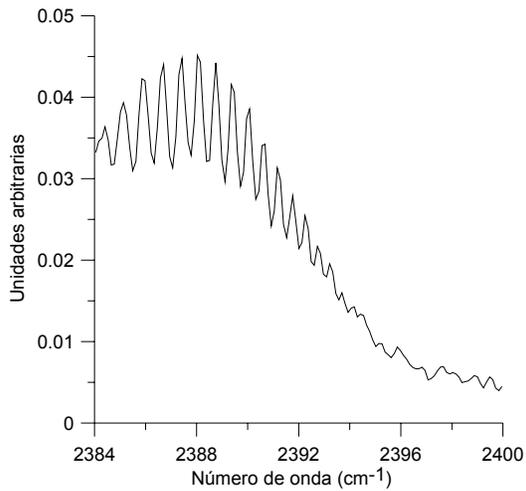


Figura 6.6. Espectro de emisión (izquierdo) y termo-imagen del escape del turborreactor RR (lado derecho) durante la medición de un espectro a alta resolución en una posición. En esta ocasión la calidad en el espectro de emisión del CO_2 fue notoria. La velocidad del turborreactor durante la medición fue de 20000 RPM.

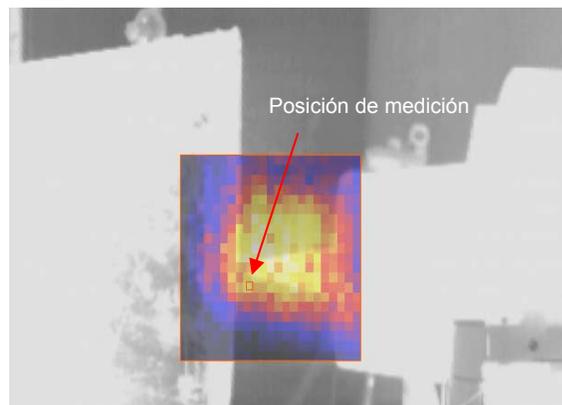
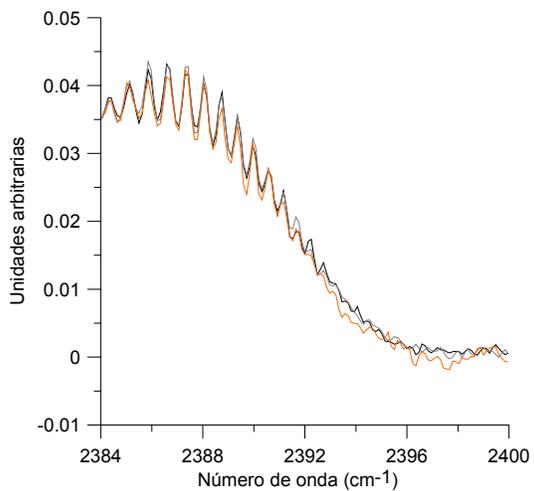


Figura 6.7. Espectros de emisión (izquierdo) y termo-imagen del escape del turborreactor RR (lado derecho) durante la medición de dos espectros a alta resolución en una posición. La calidad del espectro de emisión de CO_2 empeoró respecto a la posición pasada (note la intensidad de las líneas de emisión). La velocidad del turborreactor durante la medición fue de 20000 RPM.

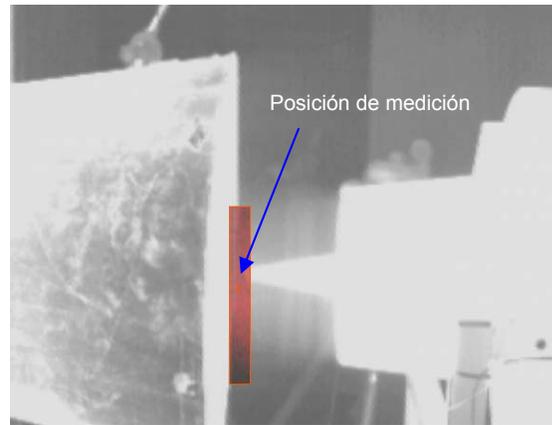
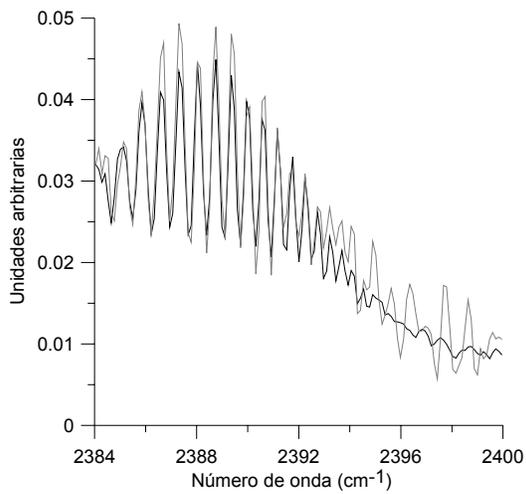


Figura 6.8. Espectros de emisión (izquierdo) y termo-imagen del escape del turborreactor RR (lado derecho) durante la medición de dos espectros a alta resolución en una posición. El espectro en color azul presenta una mejor forma debido que durante la medición de este la turbina tuvo un paro repentino por fallas técnicas. La velocidad del turborreactor durante la medición fue de 21000 RPM.

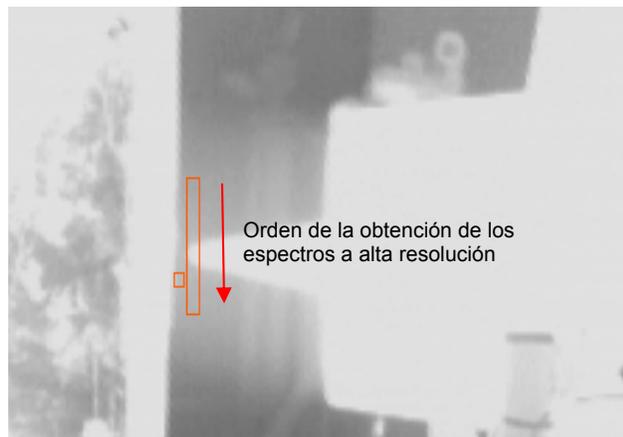
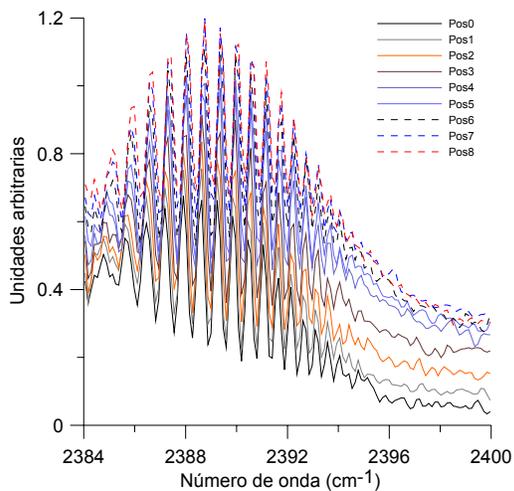


Figura 6.9. Espectros de emisión (izquierdo) y termo-imagen del escape del turborreactor RR (lado derecho) durante la medición de 8 espectros a alta resolución en orden vertical. En cada uno de los espectros puede observarse la mejoría en la calidad en las líneas de emisión del CO_2 (2384 a 2396) respecto a las mediciones anteriores. La velocidad del turborreactor durante la medición fue de 21000 RPM.

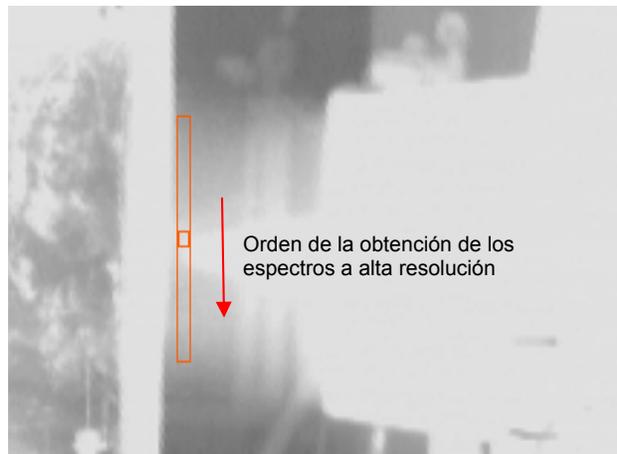
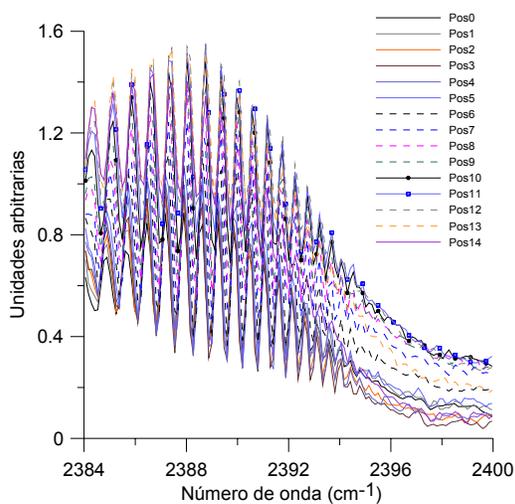


Figura 6.10. Espectros de emisión (izquierdo) y temo-imagen del escape del turborreactor RR (lado derecho) durante la medición de 16 espectros a alta resolución en orden vertical. En cada uno de los espectros puede observarse mejor calidad en las líneas de emisión del CO_2 respecto a las mediciones anteriores. La velocidad del turborreactor durante la medición fue de 19000 RPM.

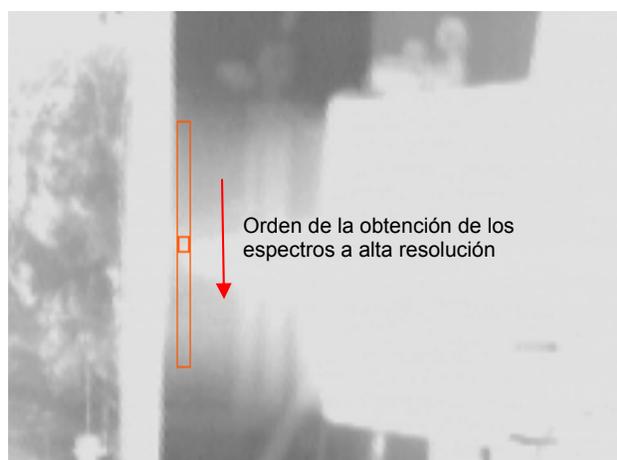
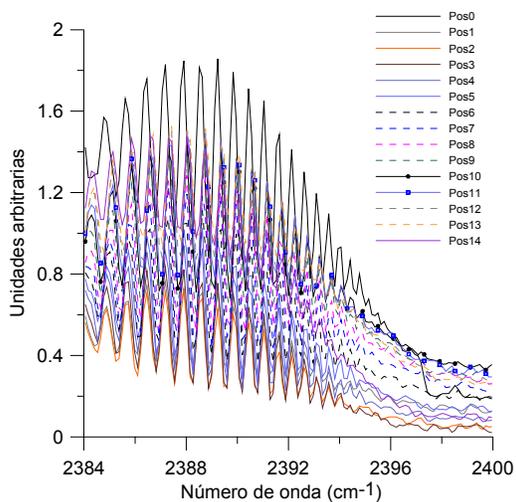


Figura 6.11. Espectros de emisión (izquierdo) y temo-imagen del escape del turborreactor RR (lado derecho) durante la medición de 16 espectros a alta resolución en orden vertical. La velocidad del turborreactor durante la medición fue de 22500 RPM.

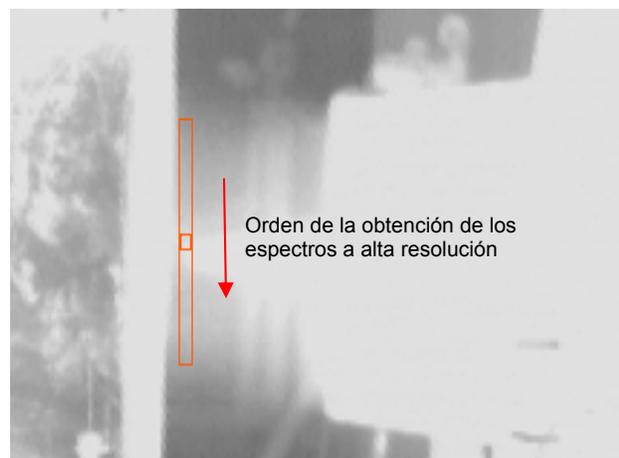
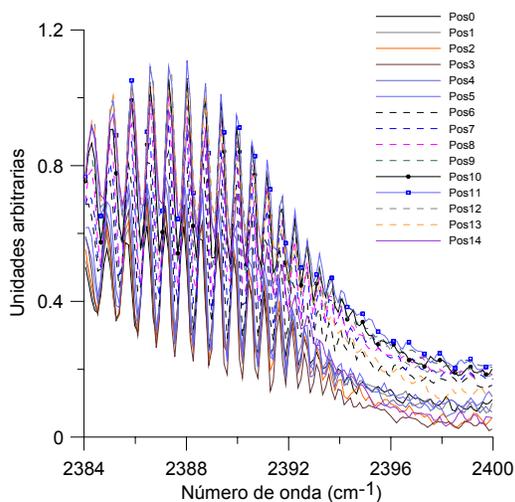


Figura 6.12. Espectros de emisión (izquierdo) y temo-imagen del escape del turborreactor RR (lado derecho) durante la medición de 16 espectros a alta resolución en orden vertical. Los espectros resultaron, al igual que en las mediciones anteriores, de buena calidad y el análisis cuantitativo de estos es mostrado en la siguiente sección. La velocidad del turborreactor durante la medición fue de 20000 RPM.

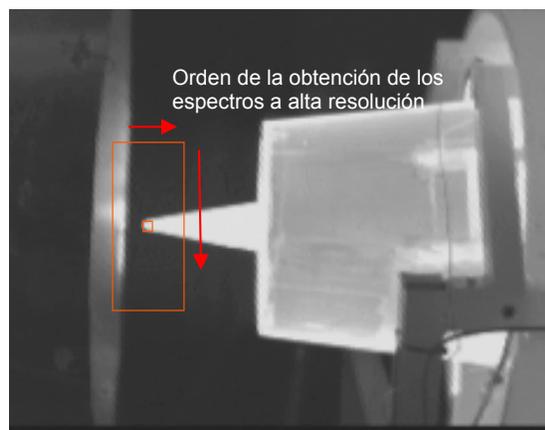
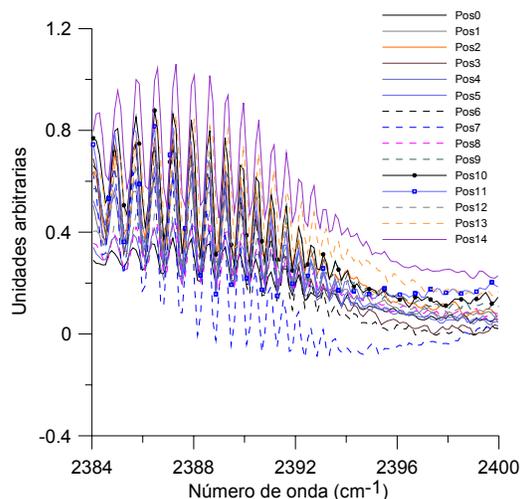


Figura 6.13. Espectros de emisión (izquierdo) y temo-imagen del escape del turborreactor RR (lado derecho) durante la medición de 32 espectros a alta resolución en orden vertical y horizontal. En esta medición los espectros resultaron con algunas interferencias que evitaron la cuantificación de compuestos por MAPS. La velocidad del turborreactor durante la medición fue de 20000 RPM.

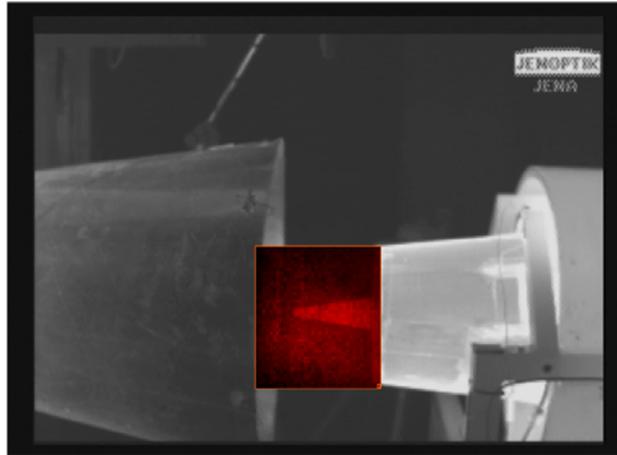


Figura 6.14. Termo-Imagen sobre puesta por falsos colores creada a través del proceso FTS programado en una secuencia vertical y horizontal. La velocidad del turborreactor durante la medición fue de 20000 RPM.

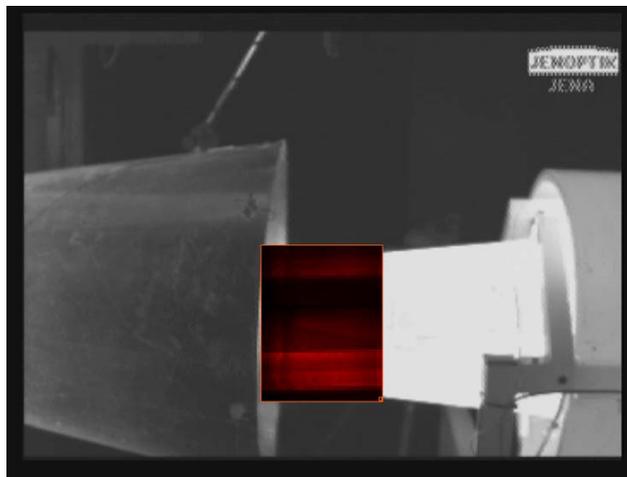


Figura 6.15. Termo-Imagen sobre puesta por falsos colores creada a través del proceso FTS programado en una secuencia vertical y horizontal. La velocidad del turborreactor durante la fue variable dentro del rango de 20000 a 10000 RPM. En la imagen puede apreciarse diferentes intensidades de color debido a los diferentes estados de potencia del quemador.

La figura 6.16 muestra en detalle la imagen obtenida por el procedimiento FTS del turborreactor operando a una velocidad de 19000 RPM. En ella son mostrados catorce espectros de emisión (a baja resolución) pertenecientes al

mismo número de posiciones en la pluma de gas. En cada uno de los espectros a baja resolución puede observarse el paulatino incremento de la intensidad de la señal en la regiones 2200 a 2300, lo cual indica un incremento en la temperatura en dichas zonas.

Posterior al procedimiento FTS, se realizó la caracterización de la distribución de la concentración de los gases de combustión NO, CO₂, CO y H₂O en la corriente de escape. La figura 6.16 a, presenta las regiones del barrido en la que fueron colectados los 16 espectros de emisión a alta resolución. Desafortunadamente de los 16 espectros originalmente colectados solo ocho pudieron ser interpretados por MAPS.

El perfil vertical de temperatura y concentración parcial obtenido a partir de la medición en dichas posiciones, con velocidades de operación de 19000 RPM y 20000 RPM, es mostrado en la figura 6.17.

El promedio de temperatura de los gases de salida á velocidades de operación de 19000 y 20000 RPM fue de 436 ± 130 °C y 353 ± 106 °C, respectivamente. Esta temperatura coincide con la reportada por un termopar instalado en la chimenea del turborreactor el cual reportó durante el experimento temperaturas de salida de los gases de 430 y 365 °C, respectivamente. El promedio de densidad de columna de CO, a 19000 y 20000 RPM, fue de $2.08 \pm 0.62 \times 10^{17}$ cm⁻² y $1.93 \pm 0.57 \times 10^{17}$ cm⁻², respectivamente.

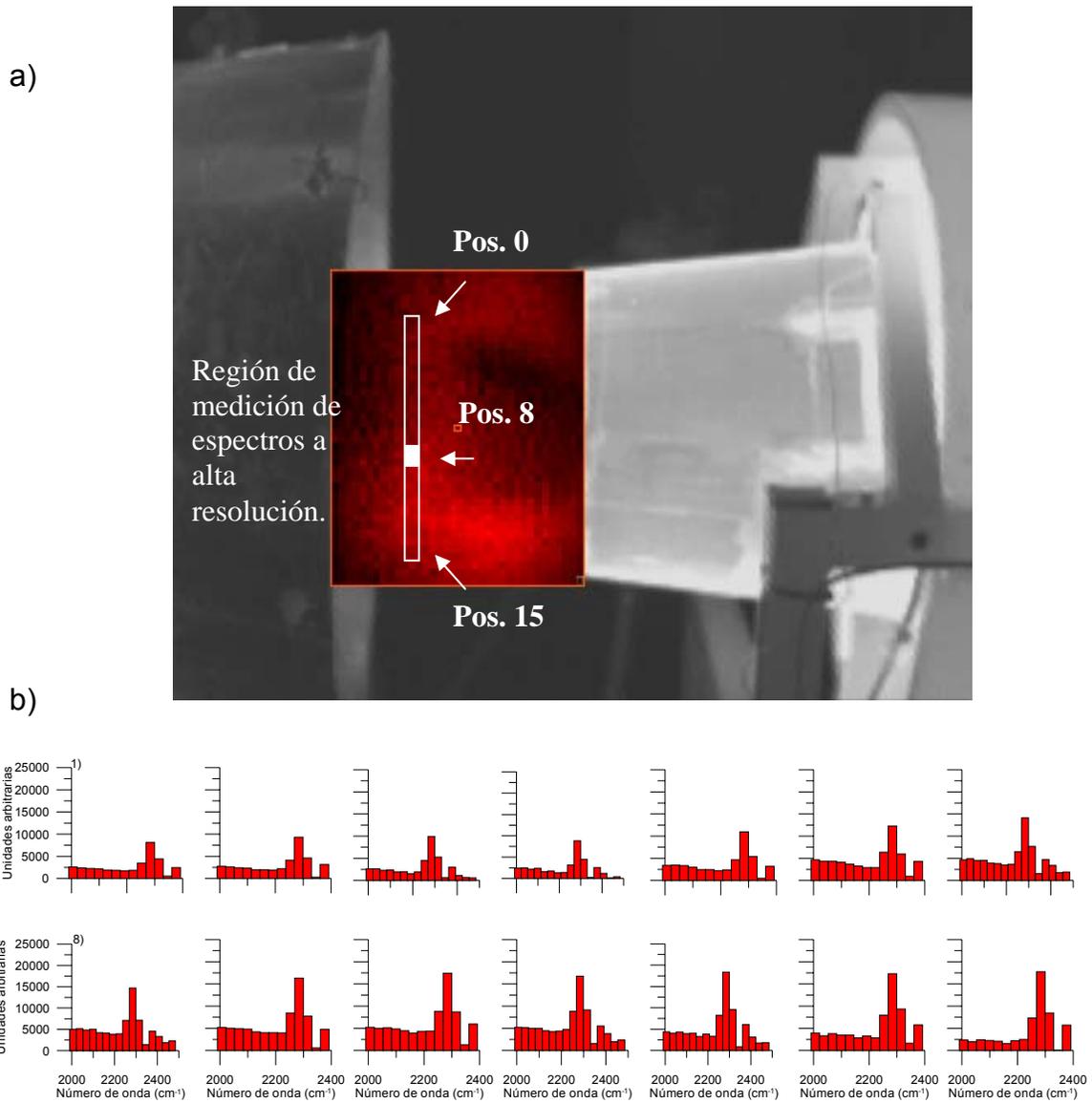


Figura 6.16 Procedimiento FTS con análisis automático de espectros. a) Imagen en colores falsos generada por el escaneo rápido de la distribución de temperatura del motor Gnome 1200 a 19000RPMs. Cada píxel de escaneo representa un espectro a baja resolución procesado por el correspondiente algoritmo de análisis. La temperatura de brillantes es proporcional al resultado numérico del algoritmo de análisis. Posteriormente el espejo fue orientado para grabar espectros a alta resolución en 8 posiciones diferentes. b) Ilustración del algoritmo usado para evaluar los espectros a baja resolución.

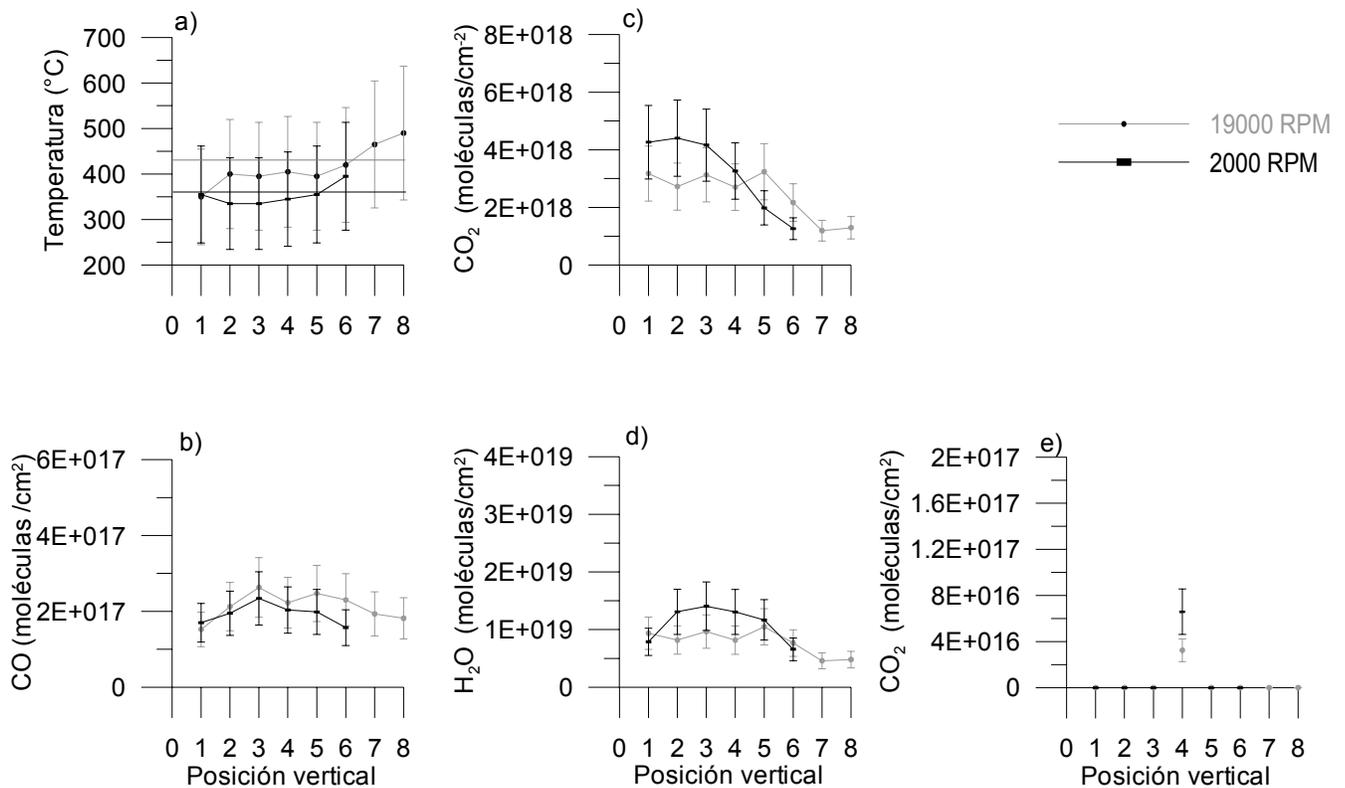


Figura 6.17. Perfil vertical de temperatura y concentración de CO, CO₂, NO y H₂O a 20000 y 19000 RPM. La barra de error para la temperatura y concertación es del $\pm 30\%$.

Los resultados de temperatura obtenidos con el espectrómetro Nicolet, del proyecto AEROTEST reportaron que la temperatura promedio calculada en ambas velocidades fue de 508 °C y de 452 °C, respectivamente. Esto resulta ser muy parecido ($\neq 70\sim 100^\circ\text{C}$) con respecto a los resultados obtenidos por el sistema SIGIS y los resultados de temperatura reportados por el termopar. De esta forma los resultados de temperatura calculados por nuestra metodología aparentemente fueron consistentes con los resultados obtenidos por el

espectrómetro del proyecto AEROTEST y por el termopar instalado en la chimenea.

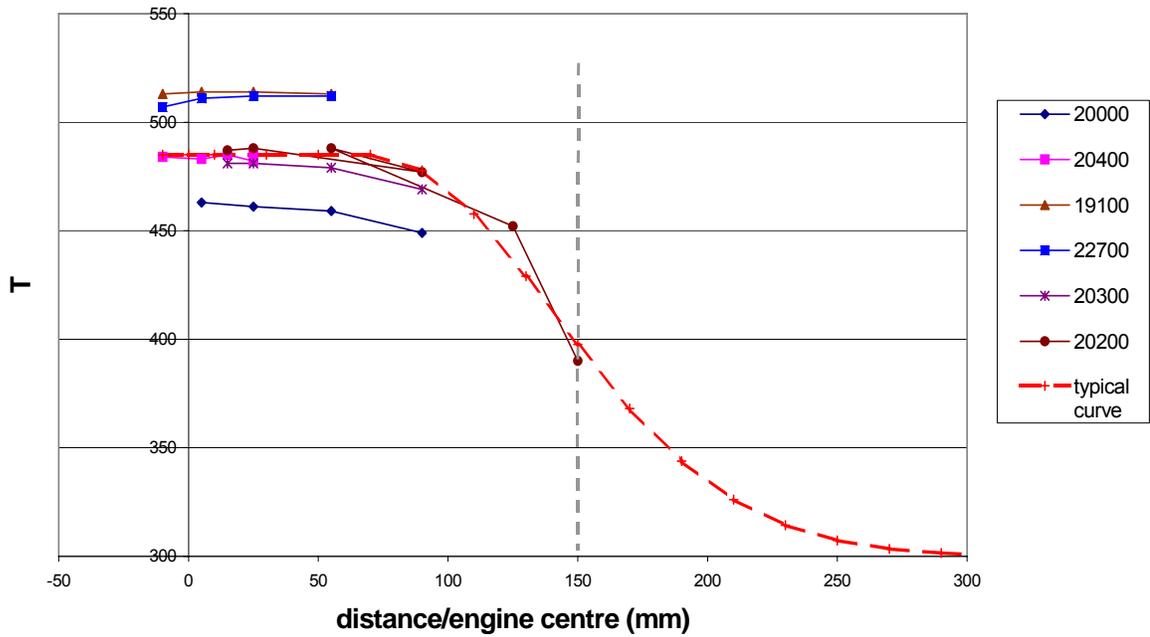


Figura 6.18. Gráfico obtenido del segundo reporte de actividades del proyecto AEROTEST en donde se muestra el perfil vertical de temperatura obtenido por el software de análisis de este proyecto a través de mediciones por percepción remota con un espectrómetro Nicolet.

CAPÍTULO

7

CONCLUSIONES

En este trabajo se contribuyó a mejorar la técnica de FTIR pasiva para la medición de emisiones de las turbinas de avión. El software MAPS fue actualizado exitosamente y con éste fueron interpretados los espectros de emisión del espectrómetro OPAG 22. La incorporación de la función de forma real del espectrómetro determinada experimentalmente mejoró la calidad de las simulaciones con respecto a los espectros medidos elevando el coeficiente de correlación entre ambos de ~ 0.7 a rangos de entre 0.94 y 0.96. Así mismo, como resultado de la investigación para evaluar dos arreglos instrumentales para ser utilizados como métodos de validación, se concluyó que a pesar de que el quemador diesel sí ofrece una corriente de gas rica en CO, CO₂ y H₂O (no así en NO), éste presenta problemas en la generación de una corriente de gas estable. Sin embargo, la celda de gases calientes resultó ser la más apropiada para la validación al comparar los resultados de las simulaciones con las condiciones controladas del experimento. Se presentan los resultados así como las recomendaciones para mejorar su diseño que serían indispensables para su implementación y estandarización. En los estudios comparativos llevados a cabo con los espectrómetros K300 y OPAG, se observó que hay consistencia en los

valores de temperatura y concentración obtenidos por ambos sistemas de medición.

En las campañas de medición llevadas a cabo en los aeropuertos internacionales de Zurich y Budapest, se pudo concluir que, a pesar de los múltiples problemas técnicos con el sistema, la visualización de los gases a través del dispositivo instalado al espectrómetro resulta altamente eficaz para la caracterización de las emisiones en aeronaves. La radiación infrarroja emitida por los gases de las turbinas a más de 40 metros de distancia pudo ser detectada y la concentración de CO, CO₂ y H₂O fue determinadas de manera remota. De igual forma, en la medición de un turborreactor instalado sobre una cama de pruebas de motores de la compañía Rolls Royce, fue posible obtener una visualización casi instantánea de la distribución de la temperatura y de los gases de combustión CO, CO₂ y H₂O emitidos por el turborreactor. En estas mediciones se observaron anomalías importantes en su distribución espacial lo que apunta a que en la caracterización de las emisiones con los métodos convencionales es sumamente importante tomar en cuenta estas variaciones fácilmente detectables con este sistema de visualización. Al comparar los resultados de temperatura calculados por con este sistema y un segundo equipo de percepción remota instalado en forma paralela, se obtuvieron datos consistentes dentro de los rangos de error de los instrumentos.

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Investigation of temperature and gas concentration distributions in hot exhausts (airplanes and burners) by scanning imaging FTIR spectrometry

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ABSTRACT

The Scanning Infrared Gas Imaging System (SIGIS) was used to perform non intrusive measurements of a Boeing 737 and a diesel powered burner (used as a hot gas producer). During the measurements it was observed that the selection of the optimal measurement positions into the plume, visualised by an infrared image from a real-time infrared camera in which the emission intensity of different field of view (FOV) positions into the plume are plotted in false colours, is possible very precisely. This enhanced considerably the probability of detection of infrared radiation emitted by a hot gas plume (e. g. from an in-service aircraft at the ground) for the objective to determine composition and temperature of the exhausts. Using this improved localization of the optimum measurement position into the hot exhaust plume the temperature and the concentrations of CO, CO₂ and NO were calculated. Additionally, the spatial distribution of gas temperature and concentrations of CO, CO₂ and NO into the exhaust plume were determined.

Keywords: non-intrusive measurement techniques, FTIR, IR camera, imaging spectrometry, aircraft exhausts

1. INTRODUCTION

The potential environmental impact of aircraft emissions and economical aspects require that engine manufacturers develop engines with lower trace gas and particle emissions, but at the same time with high efficiencies. Each new engine developed must be shown to meet the environmental requirements laid down by regulatory bodies, thus the exhaust gas measurements which accompany all stages of engine development are an essential part of this process. Within this framework, engine manufacturers stress the necessity of implementing new methodologies capable of measuring in real time key components of the engine exhaust (CO₂, CO, H₂O, NO and NO₂) which are highly dependant on the engine's operations.

In the last few years, studies using FTIR emission spectroscopy measuring aircraft engines in test beds¹ and in in-service aircrafts^{2,3,4}, have shown that this technique, when compared to conventional in-situ measurements methods that include rotating rakes, probe sampling lines, non-dispersive infra-red detectors (NDIR), chemiluminescence analysers and flame ionisation detectors (FID), all regulated by the International Civil Aviation Organization⁵, offer important advantages over the in-situ techniques:

- low operational costs,
- ease of handling,
- online measurements,
- possibility of re-analysis without affecting the data source (measured spectra),

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- no extractive sampling, thus avoiding any chemical changes which may occur within the probe and extraction system before reaching analytical equipment,
- reduces risk of engine damage,
- possibility to perform measurements of aircraft engines during real airport operations.

In this work, FTIR emission measurements were performed with the Scanning Infrared Gas Imaging System of High Resolution (SIGIS HR)⁶ to obtain the spatial distribution of the exhaust engine plume of an in-service Boeing B737 and of a diesel powered burner used as a hot gas producer.

2. EXPERIMENTAL SET-UP

Figure 1 shows the experimental set-up for the aircraft exhaust measurements during the Budapest airport campaign in October 2004. The SIGIS HR system was pointed behind the engine and the APU exhaust during the taxi way and the parking place respectively. Instead to adjust the telescope to receive the maximum signal manually (as in previous measuring campaigns), a fast temperature scan was performed by the SIGIS HR system to visualise the plume shape characteristics and to localise the position where the signal was a maximum inside a pre-selected area. This procedure reduced the time to set the measuring position to a few seconds and enhanced the probability of detection from the infrared radiation emitted by the hot exhaust plume. After the measuring position was established, a high resolution spectrum at 0.2cm^{-1} was recorded.

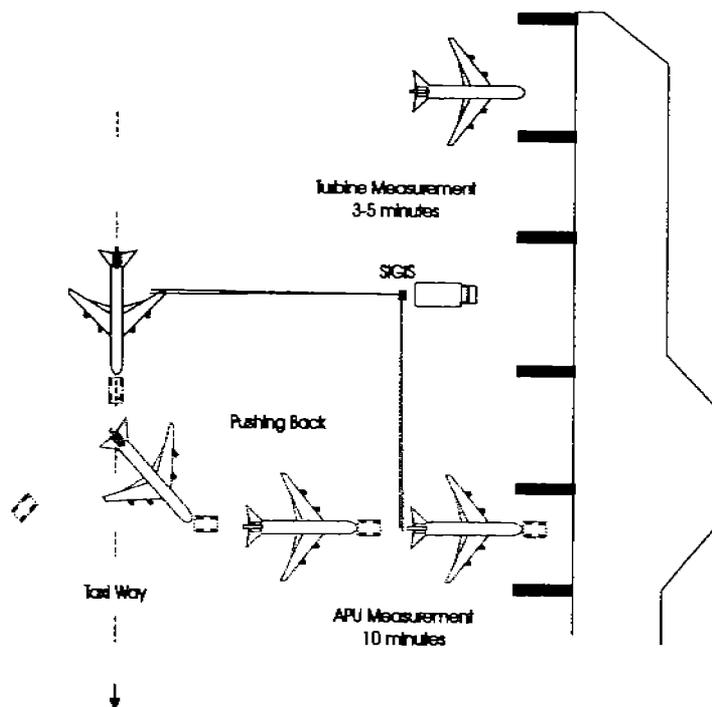


Figure 1: Scheme of the experimental set-up for measuring aircraft exhaust emissions with the SIGIS HR system at high spectral resolution. The measuring position shown allows for investigation of the aircraft situated at a parking position and on the taxiway.

3. INSTRUMENTATION

The SIGIS HR system is able to visualise the spatial distribution of the temperature of the plume by performing a two dimensional scan at different spectral resolutions. It is comprised of an OPAG 22 interferometer (Bruker) with an

operating range of between 680 and 6000 cm^{-1} (MCT detector) and a maximum spectral resolution of 0.2 cm^{-1} , an azimuth-elevation-scanning mirror actuated by stepper motors, a data processing and control system with a digital signal processor (FTIR DSP), and an image processing system (Video DSP). An IR camera coupled with the Video DSP completes the system. A full description of the instrument and its characteristics has been presented elsewhere^{6,7}.

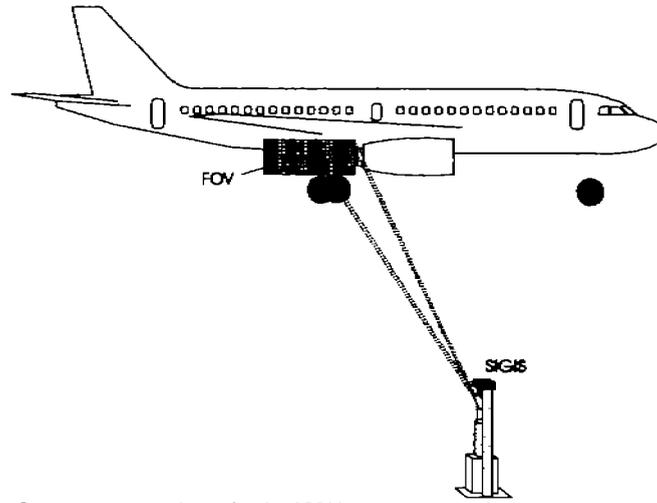


Figure 2. Example of an aircraft measurement scheme by the SIGIS HR system at the taxiway. The black rectangle corresponds to the scanned area focused by the field-of-view (FOV) from the spectrometer.

4. THE RADIATIVE TRANSFER MODEL

Basically, the propagation of monochromatic infrared radiation coming from a hot exhaust plume in the atmosphere is described by the following expression (details reference 8):

$$\frac{dI_{\sigma}}{ds} = -\beta I_{\sigma} + \beta J_{\sigma} \quad (1)$$

where I_{σ} is the intensity of radiation and β is the volume extinction coefficient that includes the contribution of the individual lines of a chemical species, is valid for monochromatic radiation and consists of two terms, the extinction represented by $-\beta I_{\sigma}$ and the emission represented by $+\beta J_{\sigma}$. For this model, the atmosphere is divided into discrete homogeneous layers in which local thermodynamic equilibrium can be assumed.

Deriving the transmission expression $\tau = \exp^{-\tau(x)}$, and introducing this in the equation (1), we can obtain the radiation that reaches the spectrometer interpreted as:

$$I_{\sigma}(2) = I_{\sigma}(1)\tau + \int_{\tau(1)}^1 J_{\sigma} d\tau \quad (2)$$

and for m th layers application:

$$I_{\sigma} = \tau_m I_{\sigma, m-1} + (1 - \tau_m) J_{\sigma}(T_m). \quad (3)$$

where $\tau_m I_{\sigma, m-1}$ represent the absorption term and $(1 - \tau_m) J_{\sigma}(T_m)$ the self radiation term of the m th layer².

4.1 Line-by-line procedure

In principle, the interpretation of the recorded spectra is done by calculating synthetic spectra at different temperatures and concentrations and then comparing them with the measured spectra by the least-squares-fitting technique. To simulate synthetic spectra, a radiative transfer model is used to describe the radiation transport of the incoming infrared radiation from a hot source into the atmosphere. The Multi-component Air Pollution Software MAPS (MAPS) is used to

interpret the spectrum recorded during the measurements and is based upon line-by-line calculations of the thermal emission and molecular absorptions of the air components.

As a first step, a quantitative analyses of the CO₂ emission spectrum is performed in the spectral window 2387 - 2397 cm⁻¹ by simulating line-by-line 19 individual transitions at different temperatures and concentrations (figure 3) using the molecular parameters extracted from the HITRAN data base. [8,9]

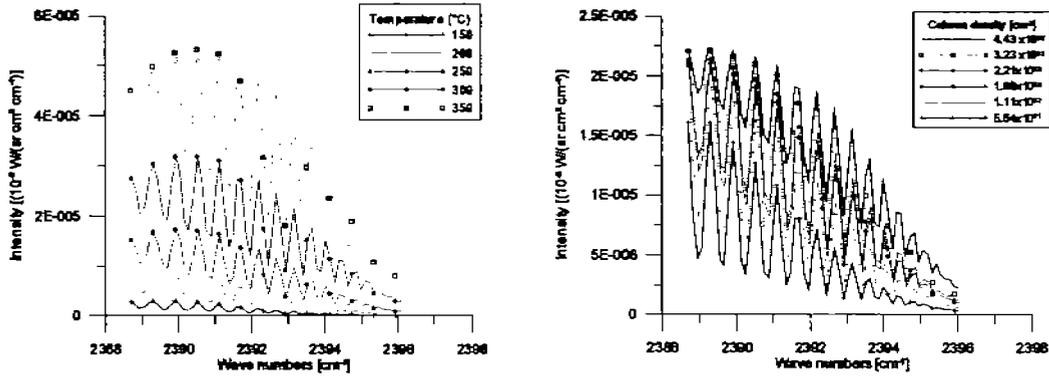


Figure 3. High resolution synthetic spectra of the CO₂ region by MAPS at six different temperature and column density levels.

Since the overall intensity of this region is dependent upon the temperature and concentration, the measured radiance is compared with the synthetic spectra, as described above, in order to provide the optimal data set.

As a second step, and with the knowledge of the plume's temperature, the concentrations in the lines around 2099 cm⁻¹ and 2169.2 cm⁻¹ are calculated for H₂O and CO, respectively. For the NO concentration evaluated at 1900.3 cm⁻¹, pre-calculated concentrations of H₂O and N₂O (at 2190 cm⁻¹) are used in the least squares procedure.

The emission index of a species X is then calculated based on the equation

$$EI(X) = EI(CO_2) \times \frac{M(X)}{M(CO_2)} \times \frac{Q(X)}{Q(CO_2)}$$

where *M* denotes the molecular weight and *Q* the concentrations (mixing ratios, column densities, etc.) of the species and *EI(CO₂)* is known from stoichiometric combustion as 3,150 g/kg.

5. EXPERIMENT

5.1 Aircraft measurements

Measurements of the CFM56-7B24 engine (Figure 4a) and the Auxiliary Power Unit (APU) of a Boeing B737 aircraft were obtained by SIGIS system (Figure 4b).

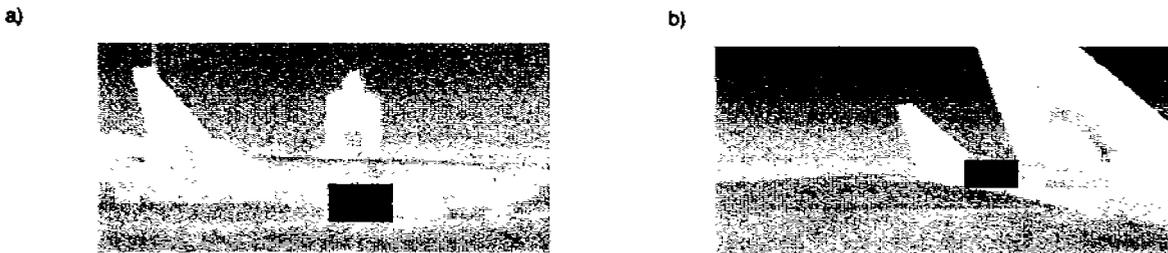


Figure 4. Thermal images from a CFM56-7B24 engine a) and an APU unit from a Boeing B737-700. The measuring position of the high resolution spectra is shown and the fast temperature scan of the turbine is represented by false colour.

The spectra from the APU and the turbines were recorded at high resolution (0.2 cm^{-1}) from a 40 and 80 m distance, respectively. The positions of the field-of-view (FOV) were selected by scanning within the area where the plume was expected, as shown in the squares of Figure 4. After simulating the infrared incoming radiation, the retrieved temperatures for the APU unit and the turbine were 290 and 390°C, respectively. Figure 5 shows the comparison of the simulated emission spectra from CO_2 at different temperatures and column densities rates.

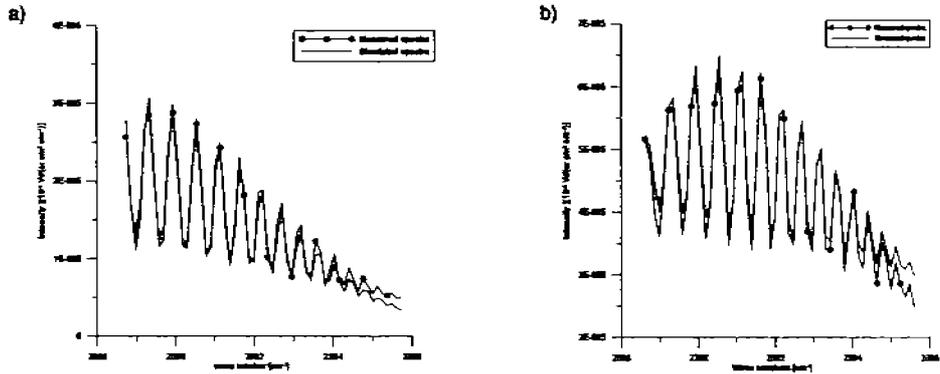


Figure 5. Comparison of two high resolution spectra measured from a) an APU and b) a turbine type CFM56-7B24 from two Boeing B737-7Q8 aircrafts and the simulated spectra from MAPS. The calculated emission indices from the APU and the turbine model CFM56-7B24 taken as the average of 3 observations are listed in the tables 1 and 2. In figure 6 and 7 the measured NO and CO emission spectra are shown, respectively.

Table 1. Emission indices from the Auxiliary Power Unit (APU) from the Boeing B737-7Q8

Compound	Calculated Emission Index
CO	22 (g/kg)
NO	0.20 (g/kg)

Table 2. Emission indices from the CFM56-7B24 engine type from the Boeing B737-7Q8 together with ICAO data.

Compound	Calculated Emission Index	ICAO reference [10]
CO	29 (g/kg)	22 (g/kg)
NO	4.21 (g/kg)	4.4 (g/kg)

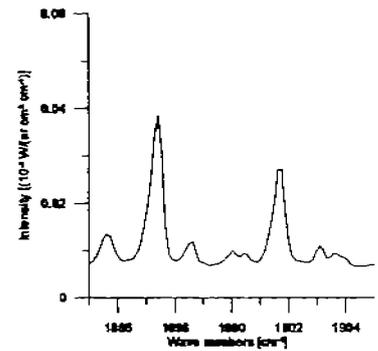


Figure 6. NO emission spectra of the turbine type CFM56-7B24 (Boeing B737) measured by the SIGIS system.

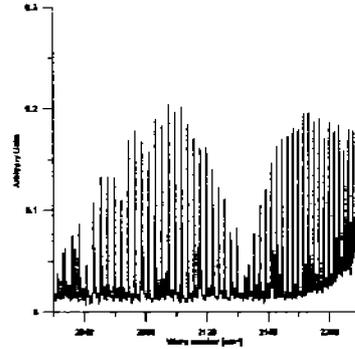


Figure 7. CO emission spectra measured by the SIGIS system from the turbine type CFM56-7B24 (Boeing B737).

5.2 Experimental set-up for the high temperature exhaust producer

With the objective to show the detection possibilities of NO emissions, a second experiment using a diesel powered burner was performed with the SIGIS system. A schematic drawing of the diesel powered burner is shown in Figure 8. The inner diameter of the steel burner tube is 50 cm and its length is 120 cm. The distance of the burner axis to the ground is about 120 cm. The burner, using diesel fuel, has a maximum power of 356 kW. The airflow inside the tube is 40,000 l/min¹³.

The SIGIS system spectrometer was placed 9.5 meters away from the burner and its telescopic mount was orientated towards the exhaust stream directly behind the burner nozzle exit. Initially, the spatial temperature distribution of the nozzle area was fast-scanned at low resolution (0.56cm⁻¹) with the SIGIS system integrated to the spectrometer to select a high resolution spectra record position.

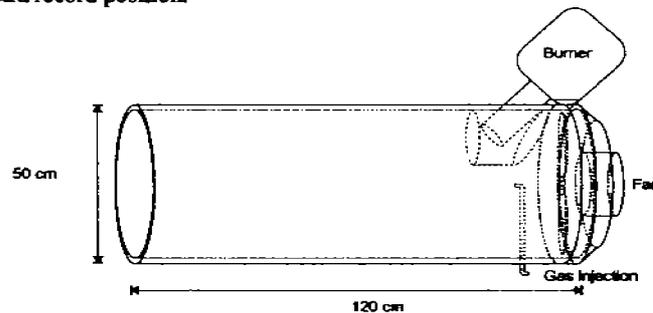


Figure 8: Sketch of the construction and dimensions of the powered diesel burner.

5.2.1 Temperature distribution

The first measurement of the plume stream was performed by a fast temperature scan which plots the temperature distribution. Figure 9 shows the scanned field of view within the plume, it is important to observe the colour contrast between different pixel positions produced principally by non homogeneous gas distribution of the hot exhaust.

To quantify the intensity of the temperature gradient in a selected area of the hot stream, the plume was divided into small homogeneous segments. Two pixel positions separated by ~10 cm were selected to record two high resolution spectra (0.2cm⁻¹). After quantitative analyse of the observed spectra, the temperature difference between both positions was found to be 320 °C and the radiation measured in the hot stream from this device was highly dependent on the relative measuring position due the non homogeneous gas distribution.

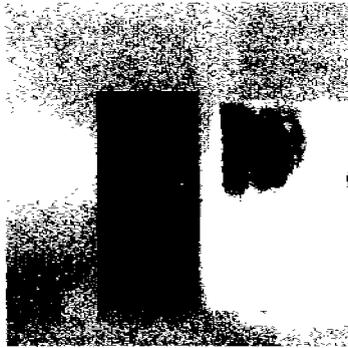


Figure 9: Infrared camera image overlapped with a low resolution scan (56cm^{-1}) for fast temperature gas identification of the diesel powered burner from a fixed position measurement.

5.2.2 Gas profile

To characterise the homogeneity of the exhaust plume¹⁴, vertical measurements were recorded from the diesel powered burner. From the quantitative gas analysis described before, the temperature and concentrations profile were obtained and are presented in figure 10. It is possible to observe an important asymmetry between the temperature and gas concentration profiles in the hot exhaust plume.

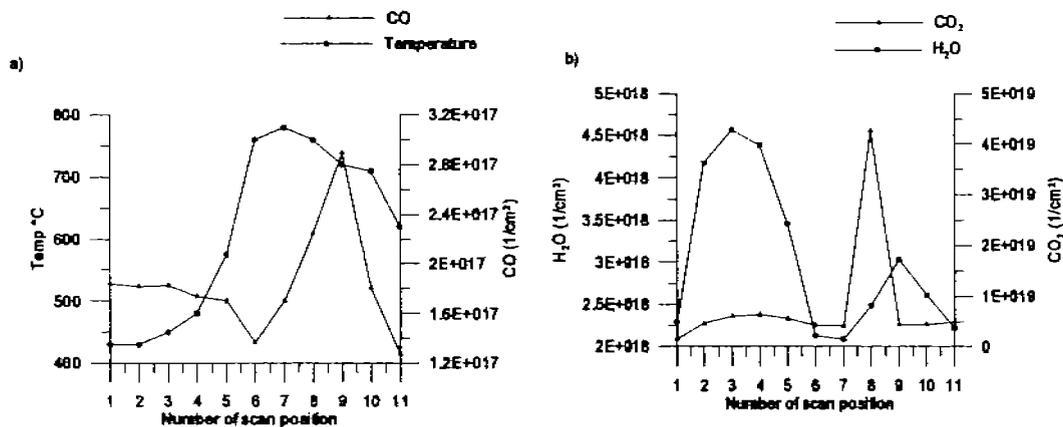


Figure 10: Spatial distribution of temperature and gas concentration of CO a) and CO₂ and H₂O b) calculated in the hot exhaust plume.

5.2.3 NO injection

Due to the low emission rate of NO gas from the diesel powered burner (lower than the detection limit), 10 L/min of pure NO was injected into this device and high resolution spectra were recorded. Different horizontal downstream positions were located using the FOV of the spectrometer by the SIGIS system (see figure 11).

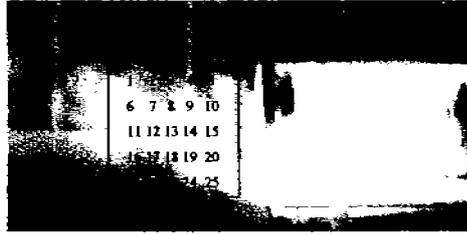


Figure 11: Infrared image of the diesel powered burner recorded during the downstream measurements. The area in the box represents the high resolution spectra record positions during the measurement.

The resultant spectrum of the measurements gave a high intensity NO signal, from which it was possible to observe differences in the NO emission lines in the recorded spectra at different field of view positions (see figure 12). After the quantitative analysis of every recorded spectrum, a temperature profile downstream from the hot exhaust plume was calculated and plotted (see figure 13).

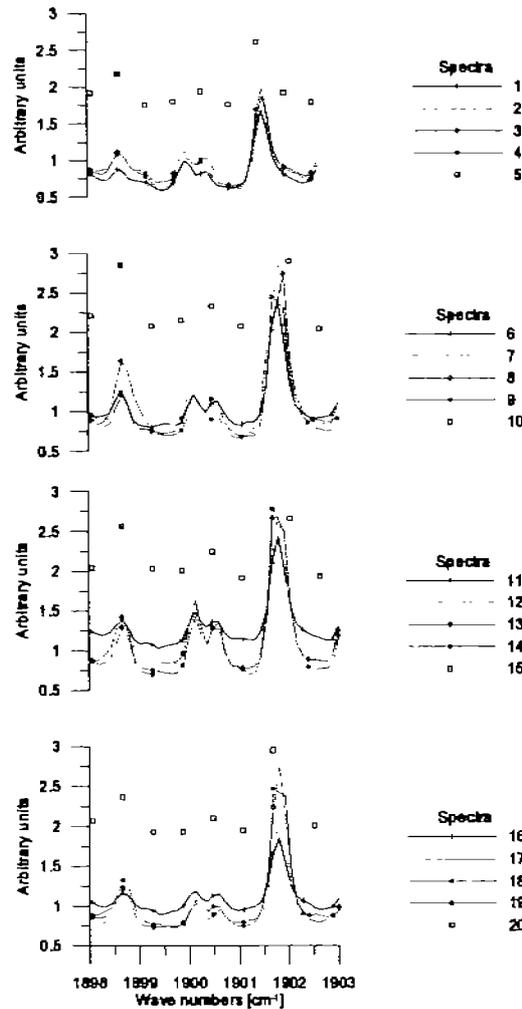


Figure 12: High spectra resolution recorded at twenty different plume positions from the diesel powered burner.

The downstream temperature profile shows a high asymmetry in the exhaust gas temperature.

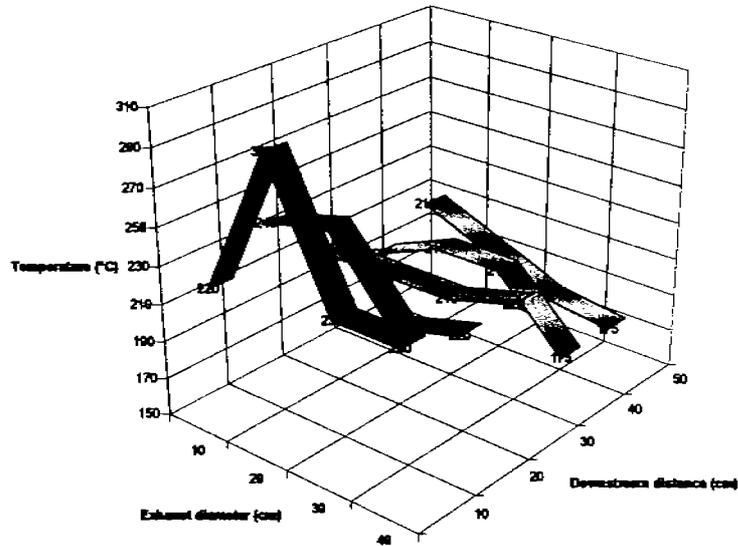


Figure 13: Temperature spatial distribution of the hot gas exhaust at four horizontal and five downstream positions.

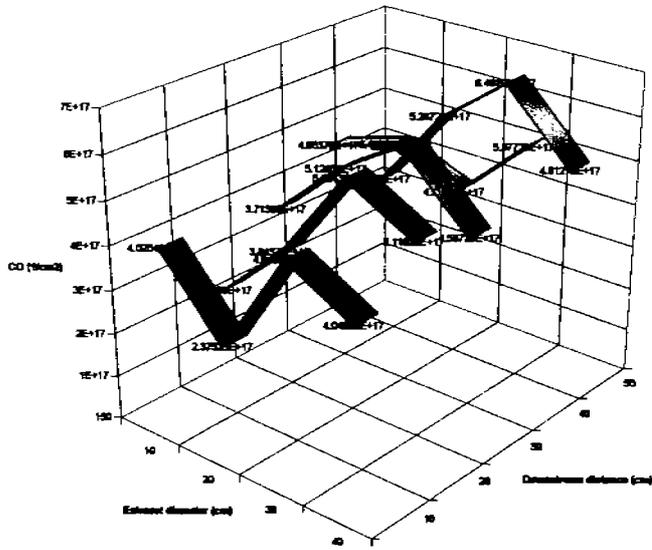
Using the infrared image recorded from the hot gas exhaust during the non-intrusive measurements, different zones were identified within the burner exhaust where the mass transfer from the hot gas stream was influenced by different effects (figure 14).



Figure 14: Infrared image from the diesel powered burner. Shows the flux behaviour of the burner powered diesel in four sections, a) represents a relative colder zone in the exhaust tube where the gas transport is relative low, b) represents the exhaust area where the hot gas stream impact the tube producing a cyclone flux, c) represents the area where is present the main gas stream and d) the zone where are present import gas vortex.

Figure 15 presents the CO and NO exhaust distribution. In the NO spatial distribution graph it is possible to observe an important inconsistency in the NO emitted rate. The NO column density is growing downstream, in theory the NO should be lower downstream due the dilution and reaction with the O_2 in to the plume, the reason for this effect is that gas streams coming from the lower exhaust part are not included in the measurements that are responsible for the fresh NO injection into the measured spectra from the selected pixels.

a)



b)

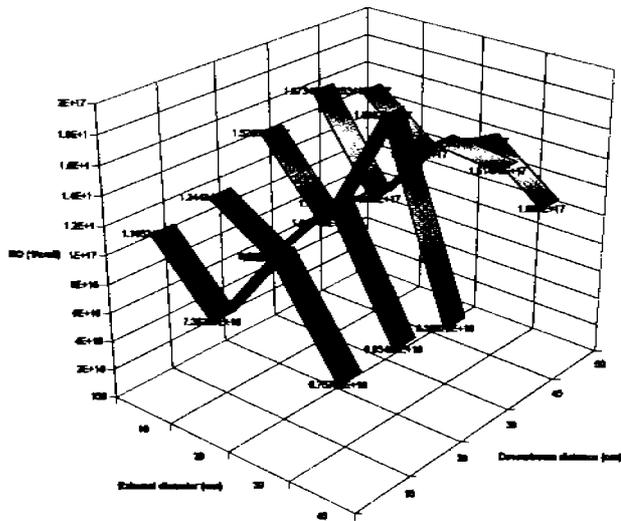


Figure 16: CO a) and NO b) spatial distribution of the hot gas exhaust at four horizontal and five downstream positions.

6. CONCLUSIONS

It has been observed that the SIGIS system enhances the probability of emissions detection, providing an important tool in the field of the FTIR emission spectroscopy.

A. Aircraft gas measurements

The gas exhaust concentrations obtained from the aircraft measurements from the turbine type CFM56-7B24 (Boeing B737) presented an increase with respect to the emissions indices reported by ICAO of 31% for CO. This difference has been also observed into the emission indices reported for different engine aircrafts in previous investigations⁴. These results show that the measurements done with the SIGIS system and the analytical software MAPS for in-work aircraft conditions can be highly reliable and the technique enhanced.

B. Hot gas producer measurements

Although the emission indices given by our hot gas producer presented low reproducibility due the technical characteristics of our device, a hot gas stream was obtained in which it was possible to inject pure NO and CO in different flux rates. All this effort had as objective to observe the detectivities of the SIGIS system and the analytical software (MAPS) to obtain detailed information from different segments inside the hot exhaust plume.

The emission spectra after scanning 11 vertical positions inside the hot exhaust plume showed well defined and strong CO spectra intensity for every one of the measure positions, giving as result a particular vertical profile of temperature that had as characteristics a non-homogeneous spatial distribution. Also from the downstream scan in 4 horizontal levels after injection of pure NO (10 l/min) a high intensity NO signal was observed into the resultant spectrum where important differences in the NO emission lines from the recorded spectra at different measurement positions were present. This enabled the production of a downstream profile of NO of the hot exhaust plume. This was also done for temperature and CO concentration.

For all these results the application of the SIGIS system and the software MAPS showed the advantages and disadvantages of a hot gas producer aircraft engine exhaust investigations and evaluation of plume models (see also¹²).

7. ACKNOWLEDGEMENTS

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Non-intrusive measurements of aircraft exhausts at airports

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Kurzfassung:

Mithilfe von Infrarot-Spektrometern werden die Emissionen von APUs (Auxiliary Power Units) sowie von Triebwerken beim Anlassen bzw. Wegrollen vom Terminal untersucht. Damit wird die quantitative Zusammensetzung des jeweiligen Abgases bestimmt. Die Spektrometer sind außerdem mit PC-gesteuerten Spiegelsystemen gekoppelt, die eine schrittweise Abtastung großer Teile der Abgasfahnen ermöglichen. So kann die Ausbreitung der Abgasfahnen und ihre Vermischung mit der Umgebungsluft untersucht werden. Weiterhin werden Offen-Pfad-Messungen im Bereich der Rollbahnen und am Terminal eingesetzt, um mittels inverser Modellierung die Quellstärken verschiedener Emittenten zu erfassen.

Abstract:

Emissions of APU (Auxiliary Power Units) and main engines are investigated by IR spectrometers during ignition, idle and taxiing. Using these data the exhaust composition is determined quantitatively. The spectrometers are coupled with PC operated scanners which enable a step-by-step imaging of the exhaust plumes. This provides information about the dispersion of exhaust plumes and their mixing with ambient air. Further, open-path measurements near the taxiways and the terminals are performed to determine by inverse modeling the emission source strengths of all relevant emission sources.

1. Introduction

The study of air quality requires the development of emission inventories (e.g. of CO and NO_x) of airports. There are mainly two types of sources, whose strength cannot be estimated easily. First there are moving sources like cars or aircrafts. Second, these are diffuse area or volume sources. The use of test bed measurements is a common procedure to estimate the source strength of moving sources. Regulations exist for measurements in aircraft main engine exhausts [1]. These emission indices are listed for each engine in a data base of the

International Civil Aviation Organisation (ICAO) for four different thrust levels (idle, approach, cruise and take-off). It is a common procedure to use this data base as a starting point to estimate aircraft emissions at airports and further on to study local air quality. But do these estimations correspond to real in-use source strengths? Further, the exhaust emissions of aircraft engines are of high speed. Their dynamic interaction with ambient air must be described for the application of small-scale chemistry-transport models.

To study these interactions, measurement techniques which need installations nearby or behind the aircraft cannot be applied. Moreover, the normal airport operation should remain unimpaired. Spectroscopic methods provide the possibilities for such investigations [2, 3, 4].

2. Measurement methods

The infrared radiation emitted by the hot gas can be analyzed by Fourier-transform infrared spectroscopy (FTIR) to determine the composition of the gas [3]. To fulfill this task, a new version of the scanning infrared gas imaging system (SIGIS-HR), using relatively high spectral resolution (0.2 cm^{-1}), has been developed [5] and applied [6]. The period of time for measurements on the engine exhaust gas of an aircraft on the ground is short during normal airport operations. Hence the remote sensing system has to be aligned to the exhaust gas plume quickly. For this reason the system is equipped with a scanning mirror actuated by stepper motors in order to allow fast changes of the line of sight. An infrared camera combined with a DSP-system enables automatic alignment of the system to the hot exhaust gas and tracking of a moving engine via online analysis of the infrared image. Additionally fast scans with low spectral resolution of the area around the engine-outlet can be performed. On the basis of the low resolution data the optimal direction for the exhaust gas measurement can be found using several automatic evaluation- and positioning-algorithms. After the SIGIS-HR-system has been positioned correctly it is operated in high-resolution-mode in order to quantify the target compounds.

The open-path measurement techniques to measure the concentrations of CO_2 , NO , NO_2 and CO are FTIR absorption spectrometry [3] and Differential Optical Absorption Spectroscopy (DOAS) [4]. Using these measurements inside the exhaust plume the emission indices are calculated directly [7]. If the measurements are performed nearby a taxiway or a terminal the concentration measurements and emission source strengths must be connected by the transport of the pollutants, which can be estimated using a dispersion model. The underlying idea to determine the source strength is to run the dispersion model varying the input parameters as long as needed to obtain the least possible difference of measured and modelled concentrations. The model input is then assumed to be the best estimation of the

emission rates [8]. Assuming a non-reactive pollutant, the transport and dispersion can be condensed into a set of linear equations and hence, linear algebra can be used to solve for the source strength (e.g. Singular Value Decomposition). The advantage of concentration measurements along a horizontal path by FTIR and DOAS is to reduce the degree of uncertainty regarding the horizontal dispersion. So the main interest of the modelling approach is to estimate the amount of vertical dispersion that accounts for the dilution of the pollutants.

3. Measurement results

Measurement campaigns were performed on idling aircraft at major European airports as Frankfurt (FRA), Munich (MUC), London-Heathrow (LRH), Paris Charles de Gaulle (CDG), Zuerich (ZRH), Vienna (VDD) and Budapest (BUD). Emission indices for CO and NO_x are calculated from passive and open-path measurements and compared to the values given in the ICAO database. The emission indices for CO for 36 different aircraft engine types and for NO_x (24 different engine types) are determined. It is shown that for idling aircraft CO emissions are underestimated using the ICAO database. The emission indices for NO_x determined are lower than given in the ICAO database. In addition a high variance of emission indices in each aircraft family and from engine to engine of the same engine type is found. During the same measurement campaigns the emission indices for CO and NO of 8 different auxiliary power units (APU) types are investigated [4].

Infrared camera images of main engines and APU provide a clear visible plume behaviour because the spectral range of the infrared camera contains transitions (emission lines) of CO₂ and H₂O. The plume is slightly meandering. More information is given by the scanning imaging FTIR spectrometer SIGIS HR. The plume length and diameter can be estimated [6]. The comparison of the width of the plume detected by the IR camera and the scanning system in the temperature mode shows that the IR camera is sensitive only for the hottest part of the plume.

An emission apportionment is conducted for the chemical species CO, NO and NO₂ from open-path measurements during a measurement campaign between two docks at Zuerich airport. Especially CO shows a good correlation to push-back events, whereas NO and NO₂ seems to be more sensitive on events on the handling places. With these promising results of the measurements, the inverse methods are applied and yielded half hourly mean emission indices. Emission rates for NO on the taxiway range from 4.4 up to 146 mg/s. For parking places a minimum emission rate of 1.6 mg/s is found. The maximum is 357 mg/s. The CO emission rates for taxiing aircrafts range from 0.4 up to 7.5 g/s, whereas for parking

places they are very low between 0.01 up to 0.35 g/s. For NO₂ on the taxiway, a minimum of 13 mg/s is observed. On the parking place this value is 0.25 mg/s. The maximum emission rate of 90 mg/s on the taxiway and 113 mg/s on the parking place is found.

4. Conclusions

The measurement methods and results shown improve the knowledge about the air quality at airports. Further developments are necessary to get higher accurate results.

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Method for On-Site Determination of the Instrument Line Shape of Mobile Remote Sensing Fourier Transform Spectrometers

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ABSTRACT

The method of passive remote sensing by Fourier transform spectroscopy allows the retrieval of column densities or concentrations of molecules in gas plumes such as exhaust gas plumes of aircraft or vapor plumes emitted after chemical accidents. State-of-the-art retrieval algorithms require two models: a radiative transfer model and an instrument model, the instrument line shape (ILS). The instrument line shape of real Fourier transform spectrometers (FTS) differs significantly from the instrument line shape of an ideal FTS, in particular if the instrument is optimized for high signal-to-noise ratio, which is achieved by interferometer designs with high optical throughput (étendue). The real instrument line shape may be modeled by convolution of the instrument line shape of the ideal FTS with an inherent instrument line shape describing the deviations. In this work, the inherent instrument line shape is modeled by a function which is dependent on a small number of parameters. In order to determine these parameters automatically, a new method has been developed. Spectra of a well-known gas in a gas cell are measured. The measured spectrum is approximated using a least squares fit with a model that contains the parameters of the instrument line shape. The fitting procedure is performed automatically. The instrument line shape model, the experimental setup of the method for the determination of the instrument line shape, and results of measurements using the instrument line shape are presented. In addition to the analysis of spectra with the ILS determined by the new method, analysis results obtained with an ideal instrument line shape are presented to demonstrate the negative effect of an inaccurate instrument line shape on the retrieved column density.

Keywords: Air pollution monitoring, Infrared spectroscopy, Fourier transform spectroscopy, Remote sensing, Instrument line shape

1. INTRODUCTION

The method of passive remote sensing by Fourier transform spectroscopy allows the qualitative and quantitative analysis of gas clouds in the atmosphere. Typical applications include the analysis of exhaust gas plumes of stacks, flares, aircraft engines, or vapor plumes emitted after chemical accidents^{1,2,3}. State-of-the-art quantitative retrieval algorithms require two models: a radiative transfer model and an instrument model, the instrument line

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shape (ILS). The instrument line shape of real Fourier transform spectrometers (FTS) differs significantly from the instrument line shape of an ideal FTS, in particular if the instrument is optimized for high signal-to-noise ratio, which is achieved by interferometer designs with high optical throughput (*étendue*). The real instrument line shape may be modeled by convolution of the instrument line shape of the ideal FTS with a so-called inherent instrument line shape describing the deviations. In this work, the inherent instrument line shape is modeled by a function which is dependent on a small number of parameters.

The possibility of a frequent determination of the instrument line shape is advantageous especially in the case of mobile spectrometers because the alignment of the interferometer may be altered by the transport of the system. In addition to the provision of the actual instrument line shape at the time of the measurement for the retrieval algorithm, an on-site determination of the instrument line shape is a functional test of the spectrometer. A potential degradation of the quality of the spectra may be identified quickly and measures to improve the quality may be taken immediately. However, even if it is not possible to remove the cause of a degraded instrument line shape on site, an accurately determined ILS may be used for the quantitative analysis of the spectra.

2. RADIATIVE TRANSFER MODEL

The basic characteristics of spectra measured by a passive infrared spectrometer may be described by a model in which the atmosphere is divided into plane-parallel homogeneous layers along the optical path⁴. In many cases a model with three layers is sufficient. Radiation from the background, for example the sky or a surface (background layer), propagates through the vapor cloud (cloud layer, a mixture of the cloud molecules and air), and the atmosphere between the cloud and the spectrometer (atmospheric layer). The radiation containing the signatures of all layers is measured by the spectrometer. The cloud layer and the atmospheric layer are considered homogeneous with regard to all physical and chemical properties. Application of the three layer model yields

$$L_S = (1 - \tau_a)B_a + \tau_a[(1 - \tau_c)B_c + \tau_c L_b] \quad (1)$$

for the spectral radiance at the entrance aperture of the spectrometer L_S . Here, τ_a is the transmittance of the atmosphere between the spectrometer and the cloud, B_a is the spectral radiance of a blackbody at the temperature of the atmosphere, T_a , τ_c is the transmittance of the cloud, and B_c is the spectral radiance of a blackbody at the temperature of the cloud, T_c . L_b is the radiance that enters the layer of the cloud from the background. The quantities in equation (1) are frequency-dependent. Because the scattering coefficient in the infrared spectral region is small under many measurement conditions, the contribution of scattering is neglected in this model. If the assumption of three homogeneous layers is not warranted, for example if there are strong temperature gradients within the layers, additional layers may be added.

If the temperatures of the cloud layer and the atmospheric layer are equal, equation (1) can be simplified:

$$L_S = B_a + \tau_a \tau_c (L_b - B_a). \quad (2)$$

It follows from equation (2) that in this case layers 1 and 2 may be exchanged without influence on the spectrum. The radiance difference $\Delta L = L_S - L_b$ is given by

$$\Delta L = (1 - \tau_{at} \tau_c) \Delta L_{cb}, \quad (3)$$

where $\Delta L_{cb} = B_c - L_b$ (Because a confusion in terms is unlikely, in this work the term radiance is used as a simplifying synonym for the correct term spectral radiance.).

If the spectrometer is aligned to a topographic target such as a forest or the wall of a house, the radiation entering the cloud from the background L_b contains radiation emitted by the surface and reflected radiation, i.e. ambient radiation and radiation from the sky. However, the emittance of many surfaces is high and is a slowly varying function of the frequency in the range $650 - 1500 \text{ cm}^{-1}$. In these cases, the radiance of a black body may be used as an approximation for L_b . In this work, measurements are performed with a black plate as the background, and L_b is modeled by the radiance of a black body.

3. INSTRUMENT LINE SHAPE MODEL

The spectrum $S^c(\sigma)$, calculated by Fourier transformation of the measured interferogram, may be written as

$$S^c(\sigma) = \int_{-\infty}^{\infty} S(\sigma') A(\sigma - \sigma', \sigma') d\sigma'. \quad (4)$$

Here, $S(\sigma)$ is the true spectrum, i.e. the spectrum measured with infinite optical path difference and collimated radiation. $A(\sigma, \sigma')$ is the instrument line shape (also called apparatus function) at the frequency σ' , i.e. the shape of the calculated spectrum (Fourier-transform of the interferogram) of monochromatic radiation with the frequency σ' . For an ideal interferometer operating with perfectly collimated radiation, the instrument line shape A_0 is given either by the Fourier transform of the function describing the finite movement of the mirror or the Fourier transform of the apodization function. If no apodization function is applied, the instrument line shape is given by

$$A(\sigma, \sigma') = A_0(\sigma) = 2D \text{sinc}(2\pi D \sigma), \quad (5)$$

where D is the maximum optical path difference in the interferometer and $\text{sinc}(x) = \sin(x)/x$. Here, the instrument line shape $A(\sigma, \sigma')$ is independent of σ' and the integral in equation (4) is a convolution integral.

In practice, in particular in the case of a passive remote sensing interferometer optimized for high throughput, non-paraxial rays from a finite source, which subtends a solid angle Ω at the interferometer, reach the detector, causing a broader instrument line shape and a frequency shift. In this case, the instrument line shape is given by the convolution

$$A(\sigma, \sigma') = A_0(\sigma) * A_{\text{non}}(\sigma, \sigma'), \quad (6)$$

where $A_{inh}(\sigma, \sigma')$, the inherent apparatus function¹⁰, is a function describing the effect of broadening and the frequency shift. In the case of a homogeneous source and an ideal Michelson interferometer (ideal mirrors etc.), in which the radiation leaving the interferometer is measured by a detector in the focal plane of a condenser lens (or mirror), $A_{inh}(\sigma, \sigma')$ is a rect-function (boxcar) of total width $\frac{\sigma \Omega}{2\pi}$, centered at $\Delta\sigma' = -\frac{\sigma \Omega}{4\pi}$ ^{5,6}. Steel⁷ investigated the inherent apparatus function of a simple Michelson interferometer without collimator and condenser. Genest and Tremblay investigated the impact of optical aberrations on the ILS⁸. Saarinen and Kauppinen deduced the inherent apparatus functions for the cases of a misaligned cube corner interferometer⁹ and an off-focus radiation source¹⁰. All the resulting instrument line shape functions are frequency-dependent, i.e. they are dependent on σ' . However, in a small spectral range $\Delta\sigma_{SR}$ around a particular frequency σ' , i.e. $\Delta\sigma_{SR} \ll \sigma'$ the spectrum may be approximated by a convolution of the true spectrum with the apparatus function at σ' (equation (4)):

$$S^c(\sigma) = S(\sigma) * A(\sigma, \sigma'). \quad (7)$$

The inherent apparatus functions cited are valid for special cases. They describe ideal interferometers or the impact of the considered setup (misaligned interferometer, off-focus source) on the line shape. In order to characterize the combined effects of aberrations, misalignment, nonlinear movement of the mirrors etc., empirical apparatus functions may be used. For passive remote sensing FTS measurements this has been described in reference 11. In reference 12, a method for active open-path measurements is presented. The instrument line shape may also be characterized by a function describing the distortions in the interferogram (for $\sigma' = const.$)^{13,14}. In reference 14, the Fourier transform of the ILS is approximated directly by linear interpolation between nodes in the interferogram (40 parameters).

In this work, two instrument line shape functions are applied. For the determination of the ILS, i.e. for modeling of measured spectra, an instrument line shape function, calculated using an empirical inherent apparatus function defined by the parameters $p_1..p_5$, is used¹¹:

$$A_{inh}(\sigma, \sigma') = \begin{cases} 0 & \text{for } \sigma < -p_1 \\ p_2 + p_3(\sigma + p_1)^2 & \text{for } -p_1 \leq \sigma \leq -p_4 \\ p_5 \text{rect} \left(\frac{\sigma + p_4}{p_4} \right) & \text{for } \sigma > -p_4 \end{cases} \quad (8)$$

This model contains the inherent apparatus function of the ideal Michelson interferometer illuminated by an extended homogeneous source as a limiting case and it contains an approximation for the inherent apparatus function of the interferometer without collimator and condenser. The parameter p_5 is required for normalization only. Because only a small spectral range around σ' is considered in this work, the dependence of the inherent apparatus function on σ' is neglected. Fig. 2 shows an experimentally determined instrument line shape function based on this model (equations (6) and (8)). In order to compare the results with the results obtained with an ideal instrument line shape, the calculations are also performed with an ideal instrument line shape (A_0).

4. METHOD FOR THE DETERMINATION OF THE INSTRUMENT LINE SHAPE

In order to determine the instrument line shape, a spectrum of a well-known gas sample contained in a gas cell is measured. The background is a heated black plate which is used in order to approximate the spectrum of a black body. The determination of the ILS is performed by minimization of the difference between the measured spectrum L_{meas} and a spectrum calculated using a model, L_{model} .

$$\sum_{i=1}^N (L_{\text{model}}^i - L_{\text{meas}}^i)^2 = \min \quad (9)$$

N is the number of spectral elements. The model contains two sub-models, a radiative transfer model for the radiance at the entrance aperture of the interferometer and a model describing instrument line shape.

The radiative transfer model for the setup used for the ILS determination is given by equation (3), with $\tau_{\text{at}} = 1$. In contrast to laboratory systems, a radiative transfer calculation including the emission of the gas has to be performed because the gas is positioned in front of the entrance of the interferometer and thus the radiation emitted by the gas is modulated by the interferometer and measured by the detector. In conventional laboratory systems, the sample is positioned between the interferometer and the detector and thus the radiation emitted by the gas is not modulated by the interferometer before it is detected.

If the test gas is contained in the HITRAN¹⁵ Database, absorption coefficients are calculated with the use of FASCODE¹⁶ under conditions of the standard atmosphere¹⁷. Alternatively, a measured high-resolution spectrum may be used. In order to minimize computation time, the (apparent) transmittance of the gas layer is approximated by convolution of a spectrum of the calculated transmittance (monochromatic) with the normalized ILS. The background layer is modeled using the spectral resolution of the measurement. In the case of a slowly varying background radiance, this method yields a good approximation in a small spectral range.

For the description of the fitting procedure, equation (9) may be written as

$$\sum_{i=1}^N (L_{\text{model}}^i(\sigma_i, T_1, cl_1, T_{\text{brbg}}, b_1, b_P, p_1, p_Q) - L_{\text{meas}}^i(f_c \sigma_{\text{cal}}))^2 = \min, \quad (10)$$

where T_1 is the temperature of the gas, cl_1 is the column density of the test gas, T_{brbg} is the mean of the brightness temperature of the background, and b_1, b_P are the coefficients of P functions for a baseline correction. p_1, p_P are the parameters of the ILS, σ_{cal} is the frequency (wavenumber) of spectral element i as determined by the previous frequency calibration (the starting value for frequency σ_i), f_c is the correction factor and $\sigma_i = f_c \sigma_{\text{cal}}$. The best-fit parameters are determined by the Levenberg-Marquardt method. In order to quantify unknown samples, an analogous method with fixed ILS parameters is applied.

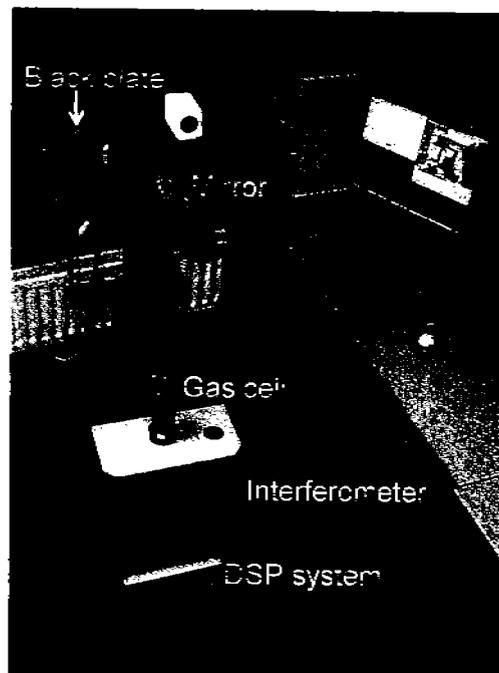


Fig. 1: Experimental setup.

5. EXPERIMENTAL DETERMINATION OF THE INSTRUMENT LINE SHAPE

All measurements were performed with the interferometer of the scanning infrared gas imaging system SIGIS^{18,19} (Bruker OPAG 22, Bruker Daltonics, Leipzig, Germany).

In order to determine the instrument line shape experimentally and to investigate the effect of the ILS on the retrieved column densities, a gas cell was mounted in front of the entrance window of the interferometer. The length of the stainless steel cell was 0.15 m, the material of the windows was NaCl. All measurements were performed with a spectral resolution of 0.5 cm^{-1} (maximum optical path difference in the interferometer: $D = 1.8 \text{ cm}$) and no apodization. The experiments were performed with ammonia. The absorption cross section of ammonia was calculated with the use of FASCODE under conditions of the standard atmosphere based on the HITRAN database. Different sample concentrations were prepared by mixing the appropriate volumes of ammonia and air in a sample bag. A heated black plate (active area $25 \times 25 \text{ cm}^2$) was used for the radiometric calibration. Moreover, the black plate was used as radiation source behind the gas cell in laboratory measurements. This setup is shown in Fig. 1. Column densities are expressed as equivalent concentration pathlength products in ppm m (288.15 K, 101325 Pa).

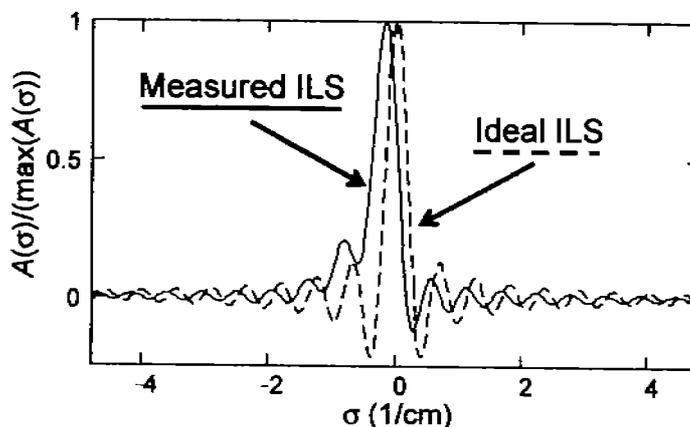


Fig. 2: Ideal instrument line shape (dashed) and measured instrument line shape (solid line).

6. RESULTS AND DISCUSSION

The instrument line shape was determined by measurement of a sample of 750 ppm m ammonia in air ($T_1 = 298$ K) in front of the black plate ($T_{bb} = 313$ K). The spectrum was recorded by averaging 16 scans of the interferometer. The model parameters were determined by application of equation (10). The resulting instrument line shape is shown in Fig. 2. It differs significantly in position, width, and symmetry from the instrument line shape of the ideal ILS which is also shown in Fig. 2.

Fig. 3 shows results of the analysis of a spectrum of 750 ppm m ammonia in air ($T_1 = 298$ K) in front of the black plate ($T_{bb} = 313$ K, single scan of the interferometer). The figure shows the results of the fitting procedure with an ideal ILS and the ILS calculated with the model (Fig. 2). Moreover, the differences are displayed for both cases. The spectrum of a blackbody at the brightness temperature of the background was subtracted.

The difference between the measured spectrum and the spectrum calculated using the model is small (Fig. 3, right), i.e. the determined instrument line shape is well-suited to approximate the real instrument line shape. The results of the fitting procedure show that the instrument line shape of the ideal FTS is not suitable for modeling the measured spectrum.

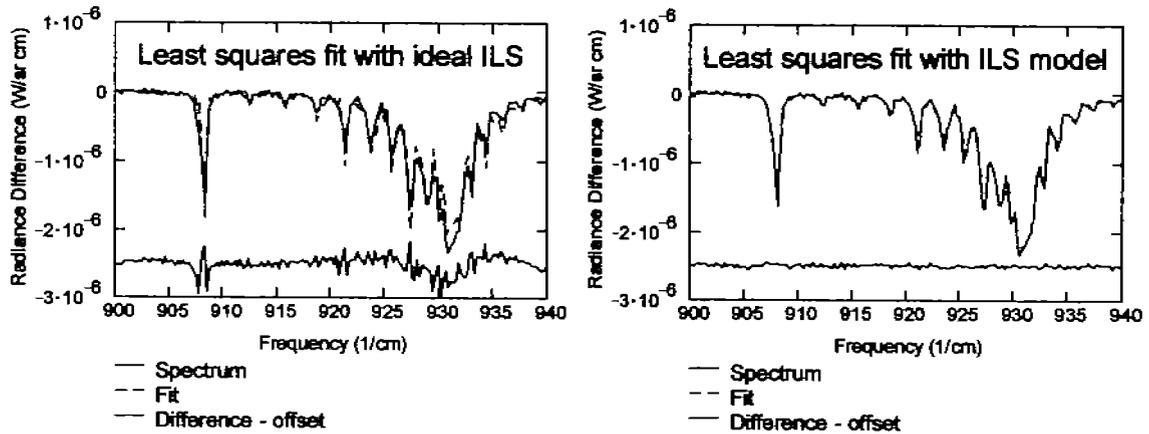


Fig. 3: Measured spectrum after subtraction of the spectrum of a blackbody at the brightness temperature of the background (solid), result of the fitting calculation (dashed). Lower curves: difference (solid, offset subtracted). Left: Results obtained with an ideal ILS (equation (5)). Right: Results obtained with the ILS model (equation (6) and equation (8)). The ideal ILS is not suitable for modeling the measured spectrum.

Fig. 4 shows results of the quantification of known samples, i.e. the retrieved column density as a function of the true column density (64 measurements, 1 scan, $T_{bb} = 313$ K). The sample temperature was room temperature (298 K). The results demonstrate the importance of a well-characterized ILS for the retrieval of the column density.

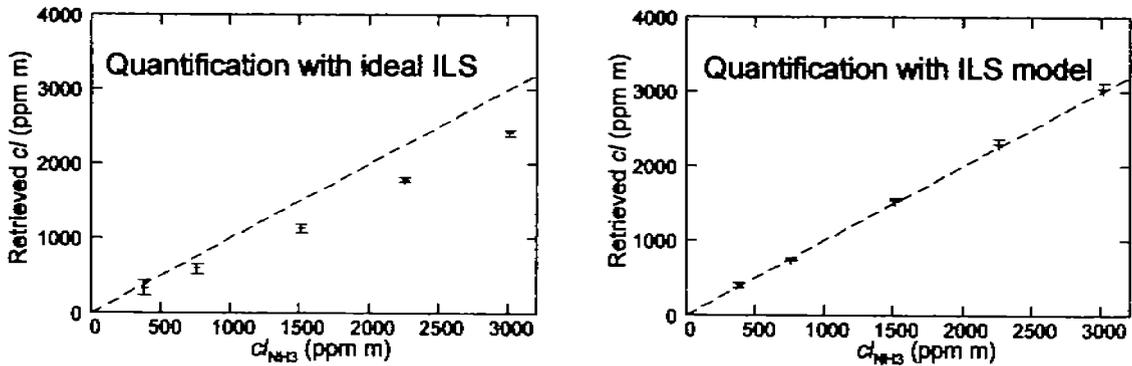


Fig. 4: Quantification by nonlinear modeling: Retrieved column density cl as a function of the true cl . Left: Results obtained with an ideal ILS (equation (5)). Right: Results obtained with the ILS model (equation (6) and equation (8)). Error bars represent standard deviations. Dashed line: $cl_{NBS} = cl_{retrieved}$.

7. SUMMARY AND CONCLUSIONS

The method presented in this work allows the determination of the instrument line shape of mobile remote sensing Fourier-transform spectrometers. The method is based on the measurement of the spectrum of a sample gas in a small gas cell. Because of this simple setup, the method is applicable on-site.

A well characterized instrument line shape is a prerequisite for accurate results of retrieval algorithms. The presented model and the ILS determined by the method described in this work allow the characterization of the instrument line shape even if the instrument is not perfectly aligned or the instrument line shape is degraded by aberrations. The negative influence on the retrieved column densities that is caused by the utilization of the instrument line shape of an ideal FTS instead of the instrument line shape determined by the method presented in this work was demonstrated.

The model for the inherent apparatus function described in this work is defined by a small number of parameters. This is possible because the model is defined by functions which are describing several distortions (finite detector area, misalignment, out of focus detector) in good approximation. The method presented in this paper is applicable to other inherent ILS models defined by parameters. Thus, if the model presented in this paper is not sufficient to describe a specific distortion, an extension of the inherent apparatus function with additional parameters is possible.

It is planned to develop a system that applies the presented method automatically by automated insertion of a short path gas cell into the optical path of the interferometer.

8. ACKNOWLEDGEMENTS

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DEVELOPMENT OF A CALIBRATION METHOD FOR FTIR SPECTROMETRY TO DETERMINE EMISSION INDICES OF HOT EXHAUSTS

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Abstract

The emissions from remote hot sources can be determined non-intrusively by FTIR spectrometry at the places of their release. One measurement mode is passive by detection of the emitted IR radiation and another active by using an IR radiation source. Temperature as well as emission indices of CO₂, CO and NO of exhausts from aircraft engines, smoke stacks and flares were determined.

Calibration methods are not available for this measurement technique. The bases for the development of corresponding guidelines were developed now. Experiments with a burner were performed. CO and NO (pure gases) were injected in the exhausts with different amounts as calibration gases to vary the concentration of these gases. The results show that this method is not accurate enough for operational use. Calibration flames and heatable calibration gas cells were investigated as comparison methods too. But also disadvantages were demonstrated for this task.

A method to determine the instrumental line shape function of the spectrometers as calibration technique will be presented.

Résumé

On peut déterminer les émissions des polluants de l'air par la spectrométrie FTIR sans accès aux sources. L'un des modes de mesure est passif. La radiation infrarouge des gaz résiduels chauds est détectée. L'autre mode est actif. La radiation infrarouge est produit par une source de radiation supplémentaire. La température et les index d'émissions de CO₂, CO et NO des gaz résiduels sont déterminés.

Il n'existe aucune méthode de calibration pour cette technique de mesure. La base pour des guides correspondants est actuellement développé. Des expériences avec un brûleur sont réalisées. CO et NO (gaz pur) sont injectés dans les gaz résiduels en différentes quantités pour varier la concentration des polluants. Le résultat indique que cette méthode n'est pas assez précise pour un usage opérationnel. Pour une

comparaison des différentes méthodes de calibration existantes, une flamme de calibration et une boîte réchauffable avec le gaz de calibration sont utilisées. Il est ainsi montré que les différentes méthodes présentent des désavantages.

Une méthode pour déterminer la fonction instrumentale de la forme de ligne (instrumental line shape function) du spectromètre est présentée.

1. Introduction

In the last few years, studies using Fourier Transform Infrared (FTIR) spectroscopy measuring aircraft engines in test beds [1] and at in-service aircrafts [2, 3, 4], have shown that this technique, when compared to conventional in-situ measurement methods that include rotating rakes, probe sampling lines, non-dispersive infra-red detectors, chemiluminescence analysers and flame ionisation detector, all regulated by the International Civil Aviation Organization [5], offer important advantages over the in-situ techniques:

- low operational costs,
- ease of handling,
- online measurements,
- possibility of re-analysis without affecting the data source (measured spectra),
- no extractive sampling, thus avoiding any chemical changes which may occur within the probe and extraction system before reaching analytical equipment,
- reduces risk of engine damage,
- possibility to perform measurements of aircraft engines during real airport operations.

Engine manufacturers stress the necessity of implementing these new non-intrusive techniques capable of measuring in real time key components of the engine exhaust (CO_2 , CO , H_2O , NO and NO_2) which are highly dependant on the engine's operations.

The method of remote sensing by FTIR spectroscopy allows the retrieval of column densities or concentrations of molecules in gas plumes such as exhaust plumes of aircraft, smoke stacks and flares or vapor plumes emitted after chemical accidents [6-11]. One measurement mode is passive by detection of the emitted IR radiation and another active by using an IR radiation source. Evaluation of these measurement results is necessary for routine application of the measurement method. Different methodologies and techniques for this task were considered [12-14]. These are: calibration burner, calibration flame, heatable calibration gas cell and determination of real instrumental line shape (ILS). Different FTIR spectrometers (FTS) as the high-resolution spectrometer K300 [7] (Kaysar-Threde GmbH, Munich, Germany) and the scanning imaging spectrometer SIGIS-HR [15] (Bruker OPAG 22, Bruker Daltonics, Leipzig, Germany) were used for measurements together with the line-by-line spectra retrieval software MAPS [2, 7]. The results are summarized in the following. It was decided to develop the last as QA/QC method.

1.1 Conclusions of calibration burner experiments

The burner was built by the IMK-IFU [14] with a diameter of the nozzle exit of 37 cm. The power of the burner is about 150 kW. Fresh air is pumped into the burner tube by a fan giving airflow inside the tube of 40,000 l/min. The temperature of the exhaust at the burner exit was from 300 up to 700 °C. A well defined and strong CO spectra intensity difference between 11 different perpendicular measurement positions in the exhaust plume of the SIGIS-HR was found. The perpendicular profile of temperature to the plume axis kept stable before and after the injection of CO (430 up to 780 °C). The measured perpendicular CO concentration profile to the plume axis before was 310 up to 783 ppmV. A strong concentration variation was found in the retrieved concentrations of CO during this experiment which was caused by wind influences

upon the exhaust plume. The comparison between the CO₂ and CO concentrations shows correlation coefficients R² of 0.41 and 0.67 for different measurement series with SIGIS-HR and K300. This shows a relevant chemical transformation of the injected CO in the exhaust plume.

65 up to 1300 ppmV of NO were injected into the burner exhaust. The maximum concentration of detected NO was 460 ppmV and it corresponds to an injection of 1300 ppmV NO. The correlation coefficient R² between measured and injected NO concentrations was 0.97 for the K300 and 0.93 for the SIGIS-HR. Enhanced NO₂ signatures were detected in the spectral window from 1628 up to 1634 cm⁻¹ for six different NO injection rates (100, 138, 230, 255, 425, and 925 ppmV). This shows a chemical transformation of the injected NO in the exhaust.

Finally, using a burner, problems with homogeneous mixing and chemical transformation of injected gases (CO, NO) were found.

1.2 Conclusions of calibration flame experiments

The measurement of the flame exhaust composition of a McKenna burner by the spectrometers K300 and SIGIS-HR shows that the repeatability of the experiment is not reliable. This is caused mainly by any small streaming of ambient air (e.g. by opening the door of the laboratory) influencing the position of the flame. If the ambient area of the flame is modified including a transparent (in the infrared) cylinder to stabilise the exhausts the quality of the results could be improved. Another possibility is the injection of CO and NO calibration gases. But in this case chemical reactions of these gases occur in the flame and the handling of the system becomes more complicated and dangerous.

Finally, calibration flames are much easier to handle than a burner but the same difficulties exist with added calibration gases.

1.3 Conclusions of heatable calibration gas cell experiments

The system for experiments with the hot cell includes a heatable cell, thermo-couples for temperature control, manometer and a regulation device. The cell was operated with a constant gas mixture in the cell during the measurement (no gas flow). Radiation emission measurements were performed with gas mixtures of 500 ppmV CO and 3 % CO₂, in synthetic air. For radiation absorption measurements a CO concentration of 2 % was used.

Heatable cell means that materials for temperatures higher than 500°C are necessary. To get the required precision is a difficult task during operational use caused by inhomogeneities of temperature and mixed gases inside the cell mainly. The disadvantages are the influences by windows and walls of the cell also.

Finally, the use of hot cells with calibration gases means a high technical effort so that this is no solution for operational use during field or test bed campaigns.

1.4 Method to determine real ILS as calibration method

The determination of the real ILS offers the possibility to check the correct optical alignment of the FTS which can cause wrong concentration results from spectra retrieval. An incorrect optical alignment of the instrument cannot be found by radiometric calibration and signal check. A method is developed for determination of instrument performance specifications for all modes of FTIR spectrometry on the basis of determination of ILS, photometric linearity, stability and noise will be followed further. This quality assurance / quality control (QA/QC) method for passive and active non-intrusive instrumentation on the basis of FTIR spectrometry will be implemented for measurement tasks of hot exhausts as e.g. in engine test beds. A detailed description of the calibration procedures is given in the following.

2. Status

State-of-the-art quantitative retrieval algorithms of passive remote sensing by FTIR spectroscopy [7, 16] require two models: a radiative transfer model and an instrument model, the ILS. The ILS of real FTS differs significantly from the ILS of an ideal FTS, in particular if the instrument is optimized for high signal-to-noise ratio, which is achieved by interferometer designs with high optical throughput (étendue). The real ILS may be modeled by convolution of the ILS of the ideal FTS with a so-called inherent ILS describing the deviations. In this work, the inherent ILS is modeled by a function which is dependent on a small number of parameters.

The possibility of a frequent determination of the ILS is advantageous especially in the case of mobile spectrometers because the alignment of the interferometer may be altered by the transport of the system. In addition to the provision of the actual ILS at the time of the measurement for the retrieval algorithm, an on-site determination of the ILS is a functional test of the spectrometer. A potential degradation of the quality of the spectra may be identified quickly and measures to improve the quality may be taken immediately. However, even if it is not possible to remove the cause of a degraded ILS on site, an accurately determined ILS may be used for the quantitative analysis of the spectra.

3. Radiative Transfer Model

The basic characteristics of spectra measured by a passive FTS may be described by a model in which the atmosphere is divided into plane-parallel homogeneous layers along the optical path [17]. In many cases a model with three layers is sufficient. Radiation from the background, for example the sky or a surface (background layer), propagates through the plume (cloud or plume layer, a mixture of the plume molecules and air), and the atmosphere between the plume and the spectrometer (atmospheric layer). The radiation containing the signatures of all layers is measured by the spectrometer. The plume layer and the atmospheric layer are considered homogeneous with regard to all physical and chemical properties. Because the scattering coefficient in the infrared spectral region is small under many measurement conditions, the contribution of scattering is neglected in this model. If the assumption of three homogeneous layers is not warranted, for example if there are strong temperature gradients within the layers, additional layers may be added.

4. Instrument Line Shape Model

For an ideal interferometer operating with perfectly collimated radiation, the ILS is given either by the Fourier transform of the function describing the finite movement of the mirror or the Fourier transform of the apodization function. In practice, in particular in the case of a passive remote sensing interferometer optimized for high throughput, non-paraxial rays from a finite source reach the detector causing a broader ILS and a frequency shift. In this case, the ILS is given by the convolution of the Fourier transform of the function describing the finite movement of the mirror and the inherent apparatus function [17], which is a function describing the effect of broadening and the frequency shift. In the case of a homogeneous source and an ideal Michelson interferometer (ideal mirrors etc.), in which the radiation leaving the interferometer is measured by a detector in the focal plane of a condenser lens (or mirror), the inherent apparatus function is a rectangular function (boxcar) [18, 19]. Steel [20] investigated the inherent apparatus function of a simple Michelson interferometer without collimator and condenser. Genest and Tremblay investigated the impact of optical aberrations on the ILS [21]. Saarinen and Kauppinen deduced the inherent apparatus functions for the cases of a misaligned cube corner interferometer [22] and an off-focus radiation source [23]. All the resulting ILS functions are frequency-dependent. However, in a small spectral range the spectrum may be approximated by a convolution of the true

spectrum with the apparatus function. The inherent apparatus functions cited are valid for special cases. They describe ideal interferometers or the impact of the considered setup (misaligned interferometer, off-focus source) on the line shape. In order to characterize the combined effects of aberrations, misalignment, nonlinear movement of the mirrors etc., empiric apparatus functions may be used. For passive remote sensing FTS measurements this has been described in reference 24. In reference 25 a method for active open-path measurements is presented. The ILS may also be characterized by a function describing the distortions in the interferogram [26, 27].

In this work, two ILS functions are applied. For the determination of the ILS, i.e. for modeling of measured spectra, an ILS function, calculated using an empirical inherent apparatus function defined by five parameters is used [24]. This model contains the inherent apparatus function of the ideal Michelson interferometer illuminated by an extended homogeneous source as a limiting case and it contains an approximation for the inherent apparatus function of the interferometer without collimator and condenser.

5. Method for the Determination of the Instrument Line Shape

In order to determine the ILS, a spectrum of a well-known gas sample contained in a gas cell is measured. The background is a heated black plate which is used in order to approximate the spectrum of a black body. The determination of the ILS is performed by minimization of the difference between the measured spectrum and a spectrum calculated using a model. The model contains two sub-models, a radiative transfer model for the radiance at the entrance aperture of the interferometer and a model describing ILS.

A measured high-resolution spectrum will be used for this method. In order to minimize computation time, the (apparent) transmittance of the gas layer is approximated by convolution of a spectrum of the calculated transmittance (monochromatic) with the normalized ILS. The background layer is modeled using the spectral resolution of the measurement. In the case of a slowly varying background radiance, this method yields a good approximation in a small spectral range. The best-fit parameters are determined by the Levenberg-Marquardt method. In order to quantify unknown samples, an analogous method with fixed ILS parameters is applied.

6. Experimental Determination of the Instrument Line Shape

All measurements were performed with the interferometer of the scanning infrared gas imaging system SIGIS-HR [31, 32]. In order to determine the ILS experimentally and to investigate the effect of the ILS on the retrieved column densities, a gas cell was mounted in front of the entrance window of the interferometer. The length of the stainless steel cell was 0.15 m, the material of the windows was NaCl. All measurements were performed with a spectral resolution of 0.5 cm^{-1} (maximum optical path difference in the interferometer: $D = 1.8 \text{ cm}$) and no apodization. The experiments were performed with ammonia. The absorption cross section of ammonia was calculated with the use of FASCODE under conditions of the standard atmosphere based on the HITRAN database. Different sample concentrations were prepared by mixing the appropriate volumes of ammonia and air in a sample bag. A heated black plate (active area $25 \times 25 \text{ cm}^2$) was used for the radiometric calibration. Moreover, the black plate was used as radiation source behind the gas cell in laboratory measurements.

7. Results of laboratory studies and discussion

The ILS was determined by measurement of a sample of 750 ppm m ammonia in air ($T_i = 298 \text{ K}$) in front of the black plate ($T_{bb} = 313 \text{ K}$). The spectrum was recorded by averaging 16 scans of the interferometer. The model parameters were determined by minimization of the difference between the measured spectrum and a spectrum

calculated using the model. The resulting ILS is shown in Fig. . It differs significantly in position, width, and symmetry from the ILS of the ideal ILS which is also shown in Fig. 1.

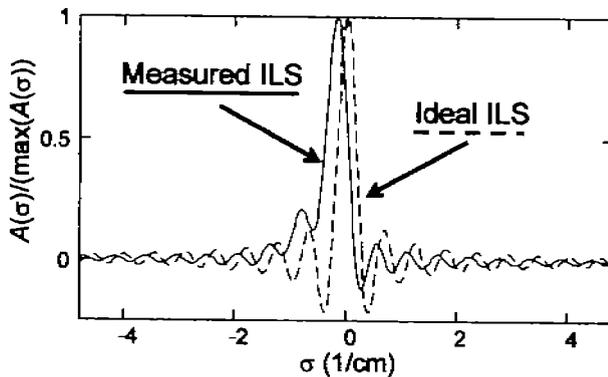


Fig. 1: Ideal ILS (dashed) and measured ILS (solid line).

The difference between the measured spectrum and the spectrum calculated using the ILS model is much smaller than that with a calculated spectrum using an ideal ILS. The results of the fitting procedure show that the ILS of the ideal FTS is not suitable for modeling the measured spectrum. This is shown in Fig. 2 where the retrieved column density of both cases is given as a function of the true column density (64 measurements, 1 scan, $T_{bb} = 313$ K). The sample temperature was room temperature (298 K). The results demonstrate the importance of a well-characterized ILS for the retrieval of the column density.

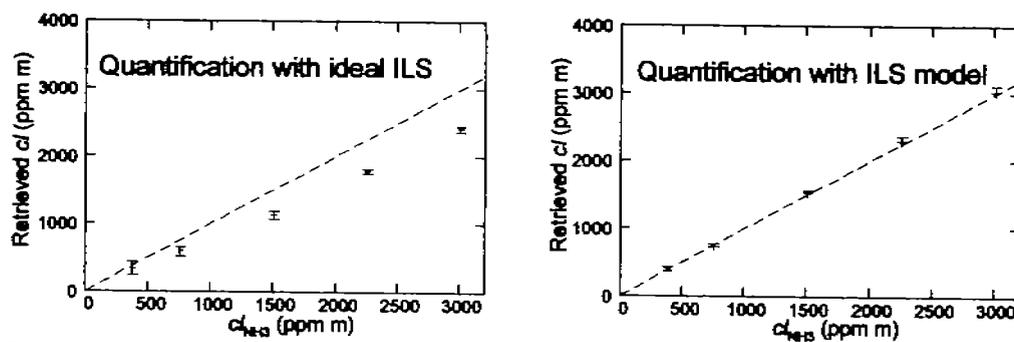


Fig. 2: Quantification by nonlinear modeling: Retrieved column density $c_{retrieved}$ as a function of the true column density c_{NH_3} . Left: Results obtained with an ideal ILS. Right: Results obtained with the ILS model. Error bars represent standard deviations. Dashed line: $c_{NH_3} = c_{retrieved}$.

8. Conclusions for further work

The method presented in this work allows the determination of the ILS of mobile remote sensing FTS. The method is based on the measurement of the spectrum of a sample gas in a small gas cell. Because of this simple setup, the method is applicable on-site.

A well characterized ILS is a prerequisite for accurate results of retrieval algorithms. The presented model and the ILS determined by the method described in this work allow the characterization of the ILS even if the instrument is not perfectly aligned or the ILS is degraded by aberrations. The negative influence on the retrieved column

densities that is caused by the utilization of the ILS of an ideal FTS instead of the ILS determined by the method presented in this work was demonstrated.

A system that applies the presented method by automated insertion of a short path gas cell into the optical path of the interferometer is under development. The typical experimental set-up for measuring the absorption spectra of gases includes a thermal radiation source, a gas cell at ambient air temperature and an interferometer. Using this set up the cell measurement won't change the configuration within the spectrometer and would provide CO absorption spectra in the exact mirror configuration used for the single emission measurements. The angle of the incoming radiation into the detector, which could produce a distortion in the paraxial rays coming from the IR source, is not changed. Further, it is not necessary for performing the ILS determination to open the spectrometer.

A stainless-steel CO gas cell will be used for the ILS determination in the case of hot exhaust gas spectral range. The optical depth of the gas cell is 2 cm and the field of view is 5 cm (see Fig. 2). BaF₂ is taken as window material and the windows are tilted by 2° to avoid reflection effects. The dimensions of the gas cell are given in Fig. 2. The inlet gas exchange is planned ones every three years.

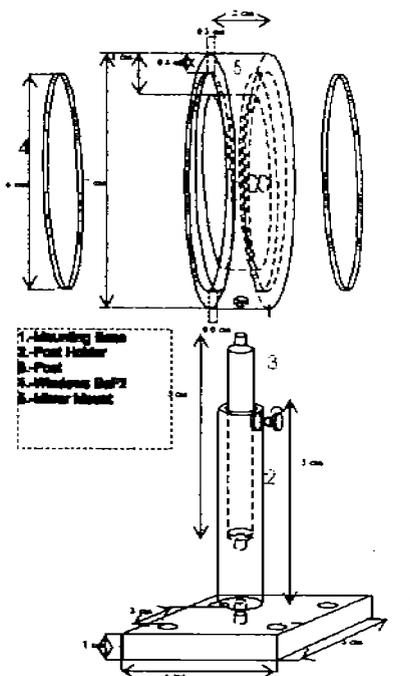


Fig. 3: Cross-section of the CO gas cell at ambient air temperature.

Before and after the engine measurements the radiation of the black body will be directed through the CO gas cell.

A software module is developed which includes the model for the inherent apparatus function and the fitting algorithm on the basis of the measured spectra with the CO cell as described before.

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Imaging scanning FTIR spectrometry to determine the composition of hot exhaust plumes

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Kurzfassung:

Die Bestimmung der Konzentrationsverteilung in Abgasfahnen ist notwendig für die Validierung numerischer Simulationen der physikalischen und chemischen Prozesse, die für die Luftbelastung in der näheren Umgebung von Bedeutung sind. Die heißen Abgase können passiv mittels FTIR-Spektrometrie erfasst und die Emissionsindizes der Abgaskomponenten bestimmt werden. Es wurden Messungen an Flugzeugturbinen in Prüfständen und auf Flughäfen durchgeführt. Dazu wurde ein FTIR-Spektrometer hoher spektraler Auflösung zur Messung der IR-Strahlung der heißen Abgase am Turbinenausgang verwendet. Zu diesem Messsystem gehört ein um 2 Achsen drehbarer Spiegel zur Erfassung der räumlichen Verteilung der IR-Strahlung der Abgasfahne. Das Spektrometer ist mit einer IR-Kamera gekoppelt, mit der das Blickfeld auf die Abgasfahne abgebildet wird.

Es werden das Messprinzip und die technische Realisierung dargestellt. Die Messergebnisse werden präsentiert und diskutiert. Es wird das Kalibrierverfahren für dieses Messverfahren auf der Basis der Bestimmung der realen instrumentellen Linienprofil-Funktion erläutert. Die Schlussfolgerungen aus diesen Ergebnissen wie u. a. der industrielle Einsatz bei Turbinen-Herstellern und die Entwicklung entsprechender Richtlinien für das Messverfahren im nationalen und internationalen Rahmen werden dargestellt.

Abstract:

The validation of numerical simulation of chemical and physical processes of hot exhaust plumes requires the determination of composition distribution. The hot exhausts can be detected passively by FTIR emission spectrometry to determine emission indices of the exhaust compounds. Measurements were performed at aircraft engines in engine test beds or at airports. A FTIR spectrometer with high spectral resolution was used to measure the IR radiation of the hot exhausts at the turbine nozzle exit. A two axis movable mirror system to image the spatial distribution of the IR radiation of the exhaust plume is part of this

measurement system. The spectrometer is coupled with an IR camera to visualise the spectrometer field of view within the exhaust plume.

The measurement principle and the technical realisation are described as well as the measurement results are presented and discussed. The calibration method of this measurement principal on the basis of the determination of the real instrumental line shape function is described. The conclusions of these results are drawn as the industrial application by turbine producers and the development of corresponding guidelines for this measurement principal in national and international scales.

1. Introduction

The validation of numerical simulation of chemical and physical processes of hot exhaust plumes requires the determination of composition distribution. Such hot exhaust plumes are of important impact for the air quality within the surrounding of such sources. These investigations are the bases for the development of measures to improve the air quality in small-scale areas as airports or industrial complexes. Emissions from remote sources as e.g. aircraft engines or chimneys of combustion processes are part of these problems.

The hot exhausts can be detected passively by FTIR emission spectrometry to determine emission indices of the exhaust compounds (CO_2 , CO , H_2O , NO and NO_2). In the last few years, studies using FTIR emission spectroscopy measuring aircraft engines in test beds [1] and in in-service aircrafts [2, 3, 4], have shown that this remote sensing technique has the ability to perform measurements similar to the regulated in situ ones by the International Civil Aviation Organization [5] but offer more flexibility during real operational conditions. In this work, FTIR emission measurements were performed with the Scanning Infrared Gas Imaging System of High Resolution (SIGIS HR) [6] to obtain the spatial distribution of the exhaust engine plume of an in-service Boeing B737.

2. Experimental set-up

To perform aircraft exhaust measurements during the Budapest airport campaign in October 2004 the SIGIS HR system was pointed behind the engine and the APU exhaust during the taxi way and the parking place respectively. Instead to adjust the telescope to receive the maximum signal manually (as in previous measurement campaigns), a fast temperature scan was performed by the SIGIS HR system to visualise the plume shape characteristics and to localise the position where the signal was a maximum inside a pre-selected area. This procedure reduced the time to set the measuring position to a few seconds and enhanced the probability of detection from the infrared radiation emitted by the hot exhaust plume. After

the measuring position was established, a high resolution spectrum at 0.2 cm^{-1} was recorded.

3. Instrumentation

The SIGIS HR system is able to visualise the spatial distribution of the temperature of the plume by performing a two dimensional scan at different spectral resolutions. It is comprised of an OPAG 22 interferometer (Bruker) with an operating range between 680 and 6000 cm^{-1} (MCT detector) and a maximum spectral resolution of 0.2 cm^{-1} , an azimuth-elevation-scanning mirror actuated by stepper motors, a data processing and control system with a digital signal processor (FTIR DSP), and an image processing system (Video DSP). An IR camera coupled with the Video DSP completes the system. A full description of the instrument and its characteristics has been presented elsewhere [6, 7].

4. Spectra Inversion

The propagation of monochromatic infrared radiation coming from a hot exhaust plume in the atmosphere is described in reference 8. In principle, the interpretation of the recorded spectra is done by calculating synthetic spectra at different temperatures and concentrations and then comparing them with the measured spectra by the least-squares-fitting technique. To simulate synthetic spectra, a radiative transfer model is used to describe the radiation transport of the incoming infrared radiation from a hot source into the atmosphere. The Multi-component Air Pollution Software (MAPS) is used to interpret the spectrum recorded during the measurements and is based upon line-by-line calculations of the thermal emission and molecular absorptions of the air components [9].

As a first step, a quantitative analyses of the CO_2 emission spectrum is performed in the spectral window $2387 - 2397\text{ cm}^{-1}$ by simulating line-by-line 19 individual transitions at different temperatures and concentrations using the molecular parameters extracted from the HITRAN data base [10, 11]. Since the overall intensity of this region is dependent upon the temperature and concentration, the measured radiance is compared with the synthetic spectra, as described above, in order to provide the optimal data set.

As a second step, and with the knowledge of the plume's temperature, the concentrations in the lines around 2099 cm^{-1} and 2169.2 cm^{-1} are calculated for H_2O and CO , respectively. For the NO concentration evaluated at 1900.3 cm^{-1} , pre-calculated concentrations of H_2O and N_2O (at 2190 cm^{-1}) are used in the least squares procedure [12].

The emission index of a species X is then calculated based on the equation

$$EI(X) = EI(\text{CO}_2) \times \frac{M(X)}{M(\text{CO}_2)} \times \frac{Q(X)}{Q(\text{CO}_2)}$$

where M denotes the molecular weight and Q the concentrations (mixing ratios, column densities, etc.) of the species and $EI(\text{CO}_2)$ is known from stoichiometric combustion as 3.150 g/kg.

5. Experiment

Measurements of the CFM56-7B24 engine (Figure 1) and the Auxiliary Power Unit (APU) of a Boeing B737 aircraft were obtained by SIGIS system. The spectra from the APU and the turbines were recorded at high resolution (0.2 cm^{-1}) from a 40 and 80 m distance, respectively. The positions of the field-of-view (FOV) were selected by scanning within the area where the plume was expected, as shown in the rectangles of Figure 1.

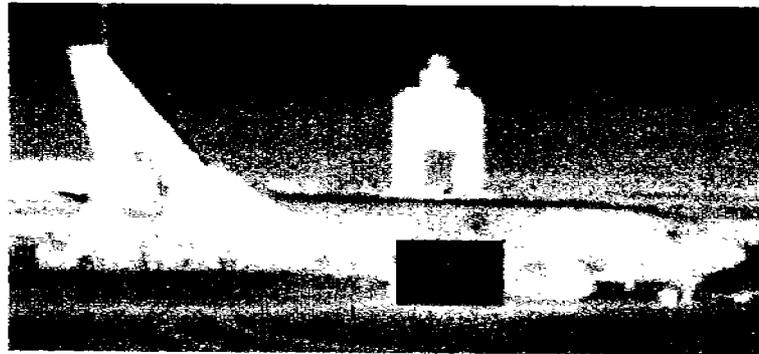


Figure 1: Thermal images by an IR camera from a CFM56-7B24 engine of a B737-7Q8. The measuring position of the high resolution spectra is shown and the fast temperature scan of the turbine is represented by false colour.

After simulating the infrared incoming radiation, the retrieved temperatures for the APU unit and the turbine were 290 and 390°C, respectively. The calculated emission indices from the APU and the turbine type CFM56-7B24 taken as the average of 3 observations are: main engines CO 29 g/kg (ICAO 22 g/kg), NO 4.21 g/kg (ICAO 4.4 g/kg); APU CO 22 g/kg, NO 0.2 g/kg.

6. Calibration method

For an ideal interferometer operating with perfectly collimated radiation, the instrumental line shape (ILS) is given either by the Fourier transform of the function describing the finite movement of the mirror or the Fourier transform of the apodization function. In practice, in

particular in the case of a passive remote sensing interferometer optimized for high throughput, non-paraxial rays from a finite source reach the detector causing a broader ILS and a frequency shift. In this case, the ILS is given by the convolution of the Fourier transform of the function describing the finite movement of the mirror and the inherent apparatus function [13], which is a function describing the effect of broadening and the frequency shift. In the case of a homogeneous source and an ideal Michelson interferometer (ideal mirrors etc.), in which the radiation leaving the interferometer is measured by a detector in the focal plane of a condenser lens (or mirror), the inherent apparatus function is a rectangular function (boxcar) [14, 15]. Steel [16] investigated the inherent apparatus function of a simple Michelson interferometer without collimator and condenser. Genest and Tremblay investigated the impact of optical aberrations on the ILS [17]. Saarinen and Kauppinen deduced the inherent apparatus functions for the cases of a misaligned cube corner interferometer [18] and an off-focus radiation source [19]. All the resulting ILS functions are frequency-dependent. However, in a small spectral range the spectrum may be approximated by a convolution of the true spectrum with the apparatus function. The inherent apparatus functions cited are valid for special cases. They describe ideal interferometers or the impact of the considered setup (misaligned interferometer, off-focus source) on the line shape. In order to characterize the combined effects of aberrations, misalignment, nonlinear movement of the mirrors etc., empiric apparatus functions may be used. For passive remote sensing FTIR spectrometer measurements this has been described in reference 20. In reference 21 a method for active open-path measurements is presented. The ILS may also be characterized by a function describing the distortions in the interferogram [22, 23].

In this work, two ILS functions are applied. For the determination of the ILS, i.e. for modeling of measured spectra, an ILS function, calculated using an empirical inherent apparatus function defined by five parameters is used [20]. This model contains the inherent apparatus function of the ideal Michelson interferometer illuminated by an extended homogeneous source as a limiting case and it contains an approximation for the inherent apparatus function of the interferometer without collimator and condenser.

6.1 Method for the Determination of the Instrument Line Shape

In order to determine the ILS, a spectrum of a well-known gas sample contained in a gas cell is measured. The background is a heated black plate which is used in order to approximate the spectrum of a black body. The determination of the ILS is performed by minimization of the difference between the measured spectrum and a spectrum calculated using a model.

The model contains two sub-models, a radiative transfer model for the radiance at the entrance aperture of the interferometer and a model describing ILS.

A measured high-resolution spectrum will be used for this method. In order to minimize computation time, the (apparent) transmittance of the gas layer is approximated by convolution of a spectrum of the calculated transmittance (monochromatic) with the normalized ILS. The background layer is modeled using the spectral resolution of the measurement. In the case of a slowly varying background radiance, this method yields a good approximation in a small spectral range. The best-fit parameters are determined by the Levenberg-Marquardt method. In order to quantify unknown samples, an analogous method with fixed ILS parameters is applied.

6.2 Experimental Determination of the Instrument Line Shape

All measurements were performed with the interferometer of the scanning infrared gas imaging system SIGIS-HR [24, 25]. In order to determine the ILS experimentally and to investigate the effect of the ILS on the retrieved column densities, a gas cell was mounted in front of the entrance window of the interferometer. The length of the stainless steel cell was 0.15 m, the material of the windows was NaCl. All measurements were performed with a spectral resolution of 0.5 cm^{-1} (maximum optical path difference in the interferometer: $D = 1.8 \text{ cm}$) and no apodization. The experiments were performed with ammonia. The absorption cross section of ammonia was calculated with the use of FASCODE under conditions of the standard atmosphere based on the HITRAN database. Different sample concentrations were prepared by mixing the appropriate volumes of ammonia and air in a sample bag. A heated black plate (active area $25 \times 25 \text{ cm}^2$) was used for the radiometric calibration. Moreover, the black plate was used as radiation source behind the gas cell in laboratory measurements.

6.3 Results of laboratory studies and discussion

The ILS was determined by measurement of a sample of 750 ppm m ammonia in air ($T_1 = 298 \text{ K}$) in front of the black plate ($T_{bb} = 313 \text{ K}$). The spectrum was recorded by averaging 16 scans of the interferometer. The model parameters were determined by minimization of the difference between the measured spectrum and a spectrum calculated using the model. The resulting ILS is shown in Figure 2. It differs significantly in position, width, and symmetry from the ILS of the ideal ILS which is also shown in Figure 2.

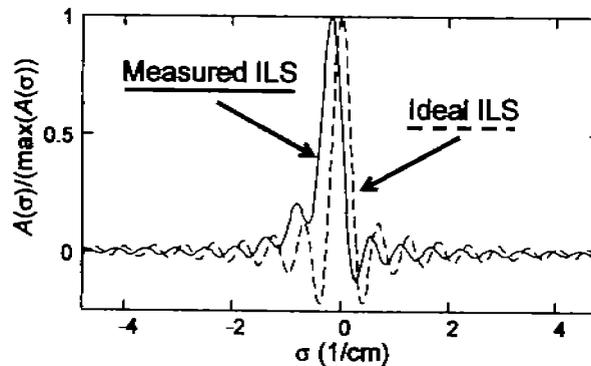


Figure 2: Ideal ILS (dashed) and measured ILS (solid line).

The difference between the measured spectrum and the spectrum calculated using the ILS model is much smaller than that with a calculated spectrum using an ideal ILS. The results of the fitting procedure show that the ILS of the ideal FTIR spectrometer is not suitable for modeling the measured spectrum (64 measurements, 1 scan, $T_{bb} = 313$ K, sample temperature 298 K). The results demonstrate the importance of a well-characterized ILS for the retrieval of the column density.

The method presented in this work allows the determination of the ILS of mobile remote sensing FTIR spectrometers. The method is based on the measurement of the spectrum of a sample gas in a small gas cell. Because of this simple setup, the method is applicable on-site.

A stainless-steel CO gas cell will be used for the ILS determination in the case of hot exhaust gas spectral range. The optical depth of the gas cell is 2 cm and the field of view is 5 cm. BaF₂ is taken as window material and the windows are tilted by 2° to avoid reflection effects. The inlet gas exchange is planned ones every three years.

7. Conclusions

It has been observed that the SIGIS HR system enhances the probability of emissions detection, providing an important tool in the field of the FTIR emission spectroscopy.

The exhaust composition obtained from the aircraft measurements of the turbine type CFM56-7B24 (B737) presented an increase with respect to the emission index reported by ICAO of 31 % for CO. This difference has been also observed into the emission indices reported for different engine aircrafts in previous investigations⁴. These results show that the measurements done with the SIGIS HR system and the analytical software MAPS for in-work aircraft conditions can be highly reliable and the technique is enhanced.

A well characterized ILS is a prerequisite for accurate results of retrieval algorithms. The presented model and the ILS determined by the method described in this work allow the characterization of the ILS even if the instrument is not perfectly aligned or the ILS is degraded by aberrations. The negative influence on the retrieved column densities that is caused by the utilization of the ILS of an ideal FTIR spectrometer instead of the ILS determined by the method presented in this work was demonstrated.

A system that applies the presented method by automated insertion of a short path gas cell into the optical path of the interferometer was developed. The typical experimental set-up for measuring the absorption spectra of gases includes a thermal radiation source, a gas cell at ambient air temperature and an interferometer. Using this set up the cell measurement won't change the configuration within the spectrometer and would provide CO absorption spectra in the exact mirror configuration used for the single emission measurements. The angle of the incoming radiation into the detector, which could produce a distortion in the paraxial rays coming from the IR source, is not changed. Further, it is not necessary for performing the ILS determination to open the spectrometer.

A software module was developed which includes the model for the inherent apparatus function and the fitting algorithm on the basis of the measured spectra with a CO cell to determine the real ILS of the spectrometer. Before and after the measurements of hot exhausts the radiation of the black body will be directed through the CO gas cell to perform the spectrometric calibration.

8. Acknowledgement

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Airport air quality studies by remote sensing of aircraft exhausts composition with passive FTIR

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ABSTRACT

The scanning infrared gas imaging system (SIGIS-HR) and the quantitative gas analysis software MAPS (Multicomponent Air Pollution Software) are applied to investigate the spatial distribution of the temperature and gas concentrations (CO, NO) within the plume of aircraft turbines at airports. The system integrates an infrared camera also. It is used for the localisation of the hot source that additionally suggests the best measurement position of the SIGIS-HR. The application of emission FTIR spectrometry for the measurement of temperature and gas emission index of CO and NO is presented for the turbine exhaust gas of a Gnome 1200 turbine. In these measurements the emitted infrared radiation of the exhaust gas stream was collected by the SIGIS-HR at different spectral resolution (56 cm⁻¹ and 0.2 cm⁻¹). Singular measurements from a Gnome 1200 turbine, originally from a Westland Wessex helicopter installed on a test bed, were done in different configurations. The software MAPS includes the Instrumental Line Shape (ILS) of the OPAG- 22 spectrometer obtained by active gas cell measurements and ILS modelling.

The rough concept of the system will be presented and operational applications will be discussed. The results of the investigations of the temperature and gas concentrations (CO, NO) within the aircraft engine plumes will be shown. The limitations and of the systems will be discussed.

Keywords: Air pollution, passive FTIR, aircraft emissions, airport emissions.

1. INTRODUCTION

In the last few years, studies using passive Fourier Transform Infrared (FTIR) spectrometry measuring aircraft engines in test beds (Schäfer et al., 2000)¹ and at in-service aircrafts at airports (Heland, Schäfer, 1997²; Heland, Schäfer, 1998³; Schäfer et al., 2003⁴), have shown that this technique, when compared to conventional in-situ measurement methods that include rotating rakes, probe sampling lines, non-dispersive infra-red detectors, chemiluminescence analysers and flame ionisation detector, all regulated by the International Civil Aviation Organization (ICAO, 1993)⁵, offer important advantages over the in-situ techniques:

- low operational costs,
- ease of handling,
- online measurements,
- possibility of re-analysis without affecting the data source (measured spectra),
- no extractive sampling, thus avoiding any chemical changes which may occur within the probe and extraction system before reaching analytical equipment,
- reduces risk of engine damage,
- possibility to perform measurements of aircraft engines during real airport operations.

Engine manufacturers stress the necessity of implementing these new non-intrusive techniques capable of measuring in real time key components of the engine exhaust (CO₂, CO, H₂O, NO and NO₂) which are highly dependant on the engine's operations.

The method of remote sensing by passive FTIR spectrometry allows the retrieval of column densities or

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concentrations of molecules in gas plumes such as exhaust plumes of aircraft, smoke stacks and flares or vapor plumes emitted after chemical accidents (Grant et al., 1992⁶; Haus et al., 1994⁷; Lindermeir, 1994⁸; Haus et al., 1998⁹; Hilton et al., 1998¹⁰; Schäfer et al., 2004¹¹). One measurement mode is passive by detection of the emitted IR radiation and another active by using an IR radiation source. Different FTIR spectrometers (FTS) as the high-resolution spectrometer K300 (Haus et al., 1994)⁷ (Kayser-Threde GmbH, Munich, Germany) and the scanning imaging spectrometer SIGIS-HR (Harig, Matz, 2001¹²; Rusch et al., 2005¹³) were used for measurements together with the line-by-line spectra retrieval software MAPS (Heland, Schäfer, 1997²; Haus et al., 1994⁷; Flores-Jardines et al., 2005¹⁴). For calibration of the measurement results the real ILS is determined. This procedure offers the possibility to check the correct optical alignment of the FTS which can cause wrong concentration results from spectra retrieval. An incorrect optical alignment of the instrument cannot be found by radiometric calibration and signal check. A method is developed for determination of instrument performance specifications for all modes of FTIR spectrometry on the basis of determination of ILS as described by Harig (2004)¹⁵. This quality assurance / quality control (QA/QC) method for passive and active non-intrusive instrumentation on the basis of FTIR spectrometry is applied (Harig et al., 2005)¹⁶. Measurements were performed at a Gnome 1200 turbine, originally from a Westland Wessex helicopter, installed on a test bed in different configurations.

The measurement method and the results of the investigations of the temperature and gas concentrations (CO, NO) within the aircraft engine plume are described in the following.

2. METHODOLOGY

2.1 Radiative transfer models

State-of-the-art quantitative retrieval algorithms of passive remote sensing by FTIR spectrometry (Goody, Yung, 1989¹⁷; Haus et al., 1994⁷; Harig, 2004¹⁵) require two models: a radiative transfer model and an instrument model, the ILS. The ILS of real FTS differs significantly from the ILS of an ideal FTS, in particular if the instrument is optimized for high signal-to-noise ratio, which is achieved by interferometer designs with high optical throughput (étendue). The real ILS may be modeled by convolution of the ILS of the ideal FTS with a so-called inherent ILS describing the deviations. In this work, the inherent ILS is modeled by a function which is dependent on a small number of parameters (Harig et al., 2005)¹⁶.

The possibility of a frequent determination of the ILS is advantageous especially in the case of mobile spectrometers because the alignment of the interferometer may be altered by the transport of the system. In addition to the provision of the actual ILS at the time of the measurement for the retrieval algorithm, an on-site determination of the ILS is a functional test of the spectrometer. A potential degradation of the quality of the spectra may be identified quickly and measures to improve the quality may be taken immediately. However, even if it is not possible to remove the cause of a degraded ILS on site, an accurately determined ILS may be used for the quantitative analysis of the spectra.

The basic characteristics of spectra measured by a passive FTS may be described by a model in which the atmosphere is divided into plane-parallel homogeneous layers along the optical path (Beer, 1992)¹⁸. In many cases a model with three layers is sufficient. Radiation from the background, for example the sky or a surface (background layer), propagates through the plume (cloud or plume layer, a mixture of the plume molecules and air), and the atmosphere between the plume and the spectrometer (atmospheric layer). The radiation containing the signatures of all layers is measured by the spectrometer. The plume layer and the atmospheric layer are considered homogeneous with regard to all physical and chemical properties. Because the scattering coefficient in the infrared spectral region is small under many measurement conditions, the contribution of scattering is neglected in this model. If the assumption of three homogeneous layers is not warranted, for example if there are strong temperature gradients within the layers, additional layers may be added (Haus et al., 1994⁷; Heland Schäfer, 1997²; Heland, Schäfer, 1998³; Schäfer et al., 2000¹).

For an ideal interferometer operating with perfectly collimated radiation, the ILS is given either by the Fourier transform of the function describing the finite movement of the mirror or the Fourier transform of the apodization function. In practice, in particular in the case of a passive remote sensing interferometer optimized for high throughput, non-paraxial rays from a finite source reach the detector causing a broader ILS and a frequency shift. In this case, the ILS is given by the convolution of the Fourier transform of the function describing the finite movement of the mirror and the inherent apparatus function (Beer, 1992)¹⁸, which is a function describing the effect of broadening and the frequency shift. In the case of a homogeneous source and an ideal Michelson interferometer (ideal mirrors etc.), in which the radiation leaving the interferometer is measured by a detector in the focal plane of a

condenser lens (or mirror), the inherent apparatus function is a rectangular function (boxcar). In a small spectral range the spectrum may be approximated by a convolution of the true spectrum with the apparatus function. In order to characterize the combined effects of aberrations, misalignment, nonlinear movement of the mirrors etc., empiric apparatus functions may be used. For passive remote sensing FTS measurements this has been described in Harig (2004)¹⁵. For the determination of the ILS, i.e. for modeling of measured spectra, an ILS function, calculated using an empirical inherent apparatus function defined by five parameters is used. This model contains the inherent apparatus function of the ideal Michelson interferometer illuminated by an extended homogeneous source as a limiting case and it contains an approximation for the inherent apparatus function of the interferometer without collimator and condenser.

2.2 Method for the Determination of the Instrument Line Shape

In order to determine the ILS, a spectrum of a well-known gas sample contained in a gas cell is measured (Harig et al., 2005)¹⁶. The radiation source is a black body. The determination of the ILS is performed by minimization of the difference between the measured spectrum and a spectrum calculated using a model. The model contains two sub-models, a radiative transfer model for the radiance at the entrance aperture of the interferometer and a model describing ILS. A measured high-resolution spectrum is used for this method. In order to minimize computation time, the (apparent) transmittance of the gas layer is approximated by convolution of a spectrum of the calculated transmittance (monochromatic) with the normalized ILS. The background layer is modeled using the spectral resolution of the measurement. In the case of a slowly varying background radiance, this method yields a good approximation in a small spectral range. The best-fit parameters are determined by the Levenberg-Marquardt method. In order to quantify unknown samples, an analogous method with fixed ILS parameters is applied.

2.3 Instrumentation

All measurements were performed with the scanning infrared gas imaging system SIGIS-HR. The SIGIS-HR is comprised of an interferometer (OPAG 22, Bruker Daltonik, Leipzig, Germany), a telescope, an azimuth-elevation-scanning mirror actuated by stepper motors, an infrared camera (Infratec, Dresden), and a data processing and control system with digital signal processors for the spectrometer and the infrared camera. In the configuration used for this study, the spectrometer has an operating range between 680 and 3500 cm^{-1} (MCT detector) and a maximum spectral resolution of 0.2 cm^{-1} . The SIGIS system is schematically shown in Figure 1.

The operational principle of the SIGIS for this application consists of placing the instrument at a safe distance from the aircraft's turbine and acquiring infrared emission spectra around the exhaust plume. The analysis, which needs to be performed while the turbine is stationary, can be done either in a test-bed or in real airport operating conditions. For completing an image of the gas plume with infrared spectral information, the scanning mirror is sequentially traversed over all positions (pixel-by-pixel) within the field view (FOV) specified by the user.

For fast visualization of the exhaust plume and brightness temperature of the background, a low-resolution mode (spectral resolution: 56 cm^{-1}) scan is performed. In this mode 17 interferograms per second are obtained and analyzed. Each interferogram is recorded by the FTIR DSP system and the signal is Fourier-transformed. The resultant spectrum is analyzed by the DSP. In order to evaluate the brightness temperature of the exhaust gas, the integral of the spectrum in a spectral range that contains emission lines of the exhaust gas is calculated (for CO_2 a typical range is 2300 - 2400 cm^{-1}). To take into account the background temperature, the spectrum is analyzed in the range 800 - 1200 cm^{-1} .

The resultant spectrum is analyzed from which the brightness temperature of the exhaust gas is evaluated. For this and in order to avoid the influence of hot parts from the engine within the field-of-view, the integral of the radiance spectrum in a spectral range that contains emission lines of the exhaust gas is calculated. The false colour images of the calculated quantities are overlaid over the images of a video or infrared camera. Because the goal of this procedure is to locate the hottest part of the gas plume and background in the FOV, only a qualitative analysis is performed, i.e. no radiometric calibration is required.

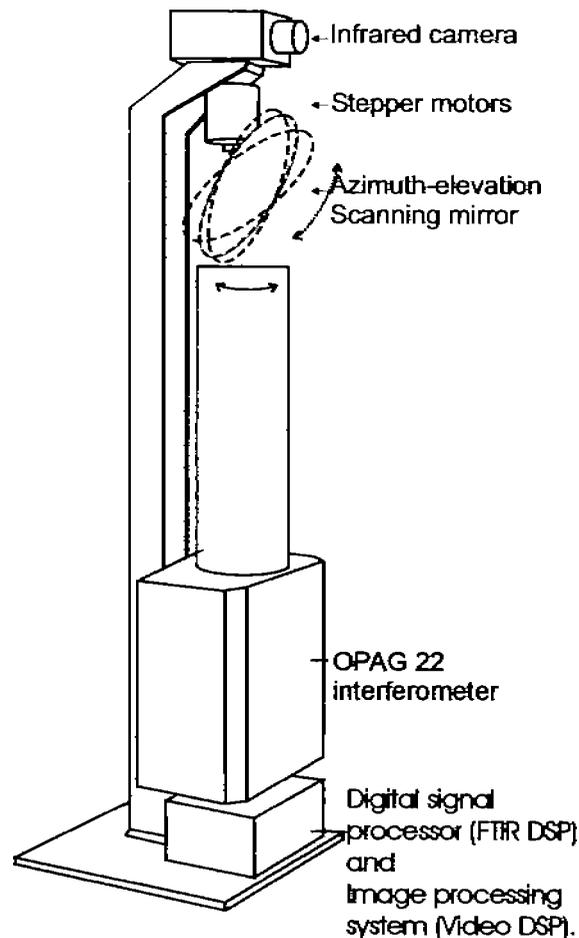


Figure 1. Schematic diagram of the Scanning Infrared Gas Imaging System (SIGIS-HR) for measuring temperature and gas distributions in turbine exhaust plumes.

Once the distribution of the brightness temperature is known, the next step is to record a high-resolution spectrum (0.2 cm^{-1}) in the position where the highest brightness temperature was detected. The spectra are averaged for at least 1 minute in order to achieve a satisfactory signal-to-noise ratio and then radiometrically calibrated against a black body at 200°C placed next to the instrument. The spectra are then further evaluated by a radiative transfer model (described below) in order to calculate the column densities of the gases.

In order to determine the ILS experimentally and to investigate the effect of the ILS on the retrieved column densities, a gas cell was mounted in front of the entrance window of the interferometer. The length of the stainless steel cell is 2 cm, the field of view is 5 cm, the material of the windows is BaF_2 and the windows are tilted by 2° to avoid reflection effects. The dimensions of the gas cell are given in Figure 2. All measurements were performed with a spectral resolution of 0.2 cm^{-1} and no apodization. The cell is filled with 2 % of CO in N_2 allowing an absorption of ~50% of the incoming infrared radiation (0.3 Absorbance units). The absorption cross section of the gas was calculated with the use of FASCODE (Smith et al., 1978)¹⁹ under conditions of the standard atmosphere (U.S. Standard Atmosphere, 1976)²⁰ based on the HITRAN database (Rothman et al., 2005)²¹. A black body of 200°C was used for the radiometric calibration. Moreover, the black body was used as radiation source behind the gas cell in laboratory measurements.

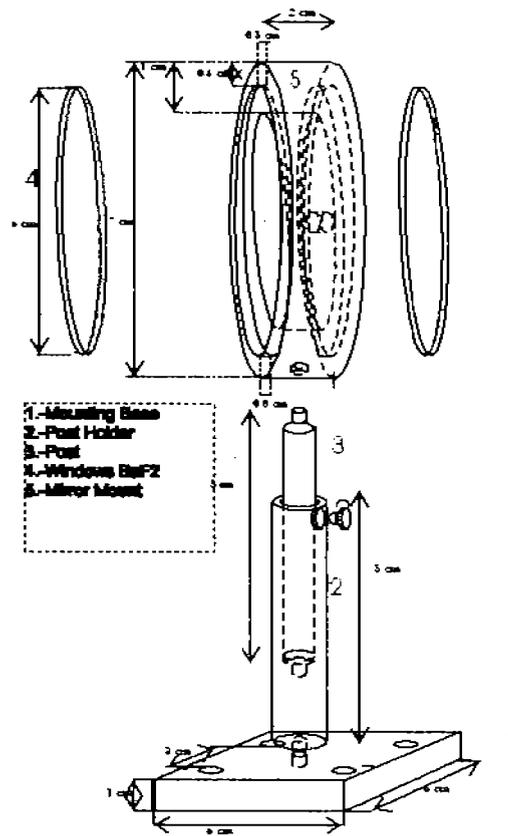


Figure 2: Cross-section of the CO gas cell at ambient air temperature.

CO gas cell spectra

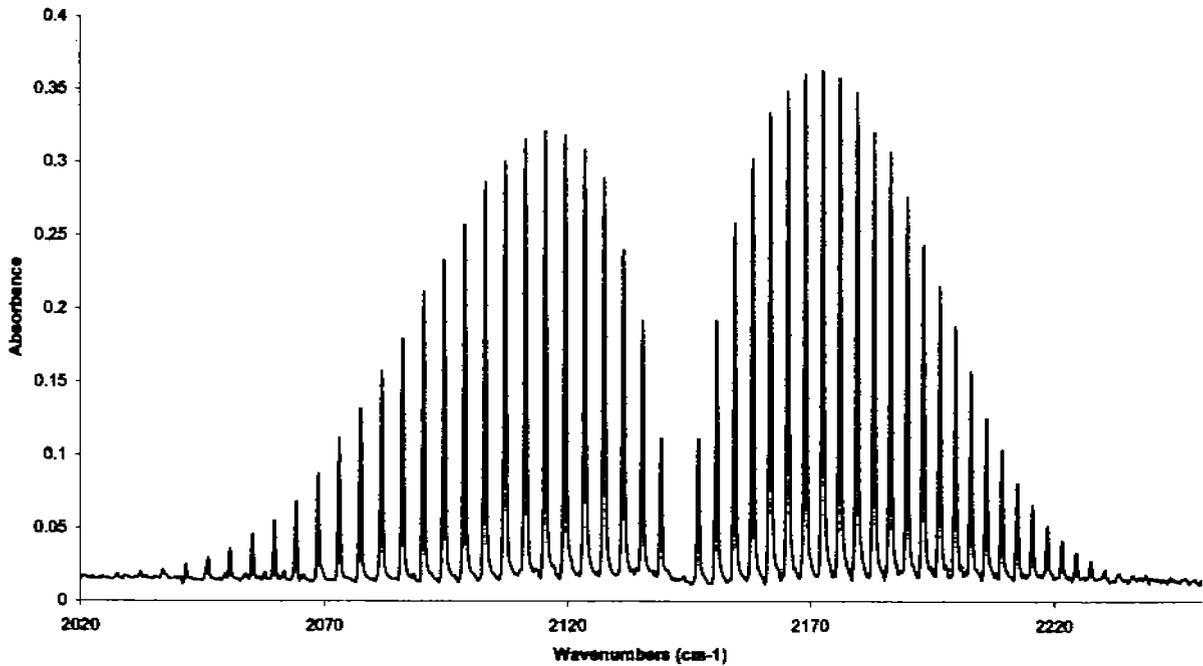
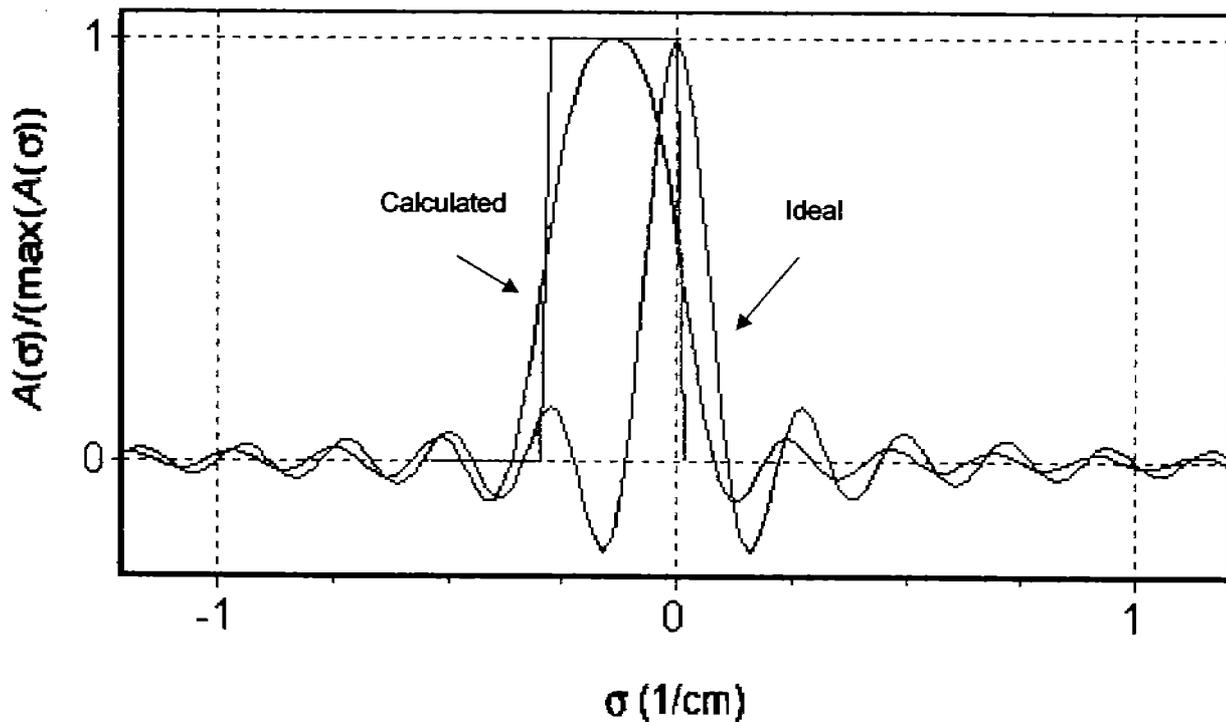


Figure 3: CO absorption spectra used for the ILS calculation.

Before and after the engine measurements the radiation of the black body is directed through the CO gas cell.

A software module was developed which includes the model for the inherent apparatus function and the fitting algorithm on the basis of the measured spectra with the CO cell as described before is developed (Harig et al., 2005)¹⁶.



Figur 4: Ideal ILS (red) and measured ILS (blue) calculated by GeDetekt software using an absorption spectrum of CO at a concentration of 20000 $\mu\text{mol/mol}$.

With the objective to observe the benefit of the inclusion of the new ILS into the software MAPS, two turbojet spectra were simulated using the original ILS (included into the first version of the software) and the new calculated ILS from the spectrometer OPAG plotted in the figure 4. As result, the observed correlation factor between the simulated and measured spectra improved in both cases from 0.73 and 0.68 (using the ILSNBS) to 0.96 and 0.94 respectively (figure 5 and 6).

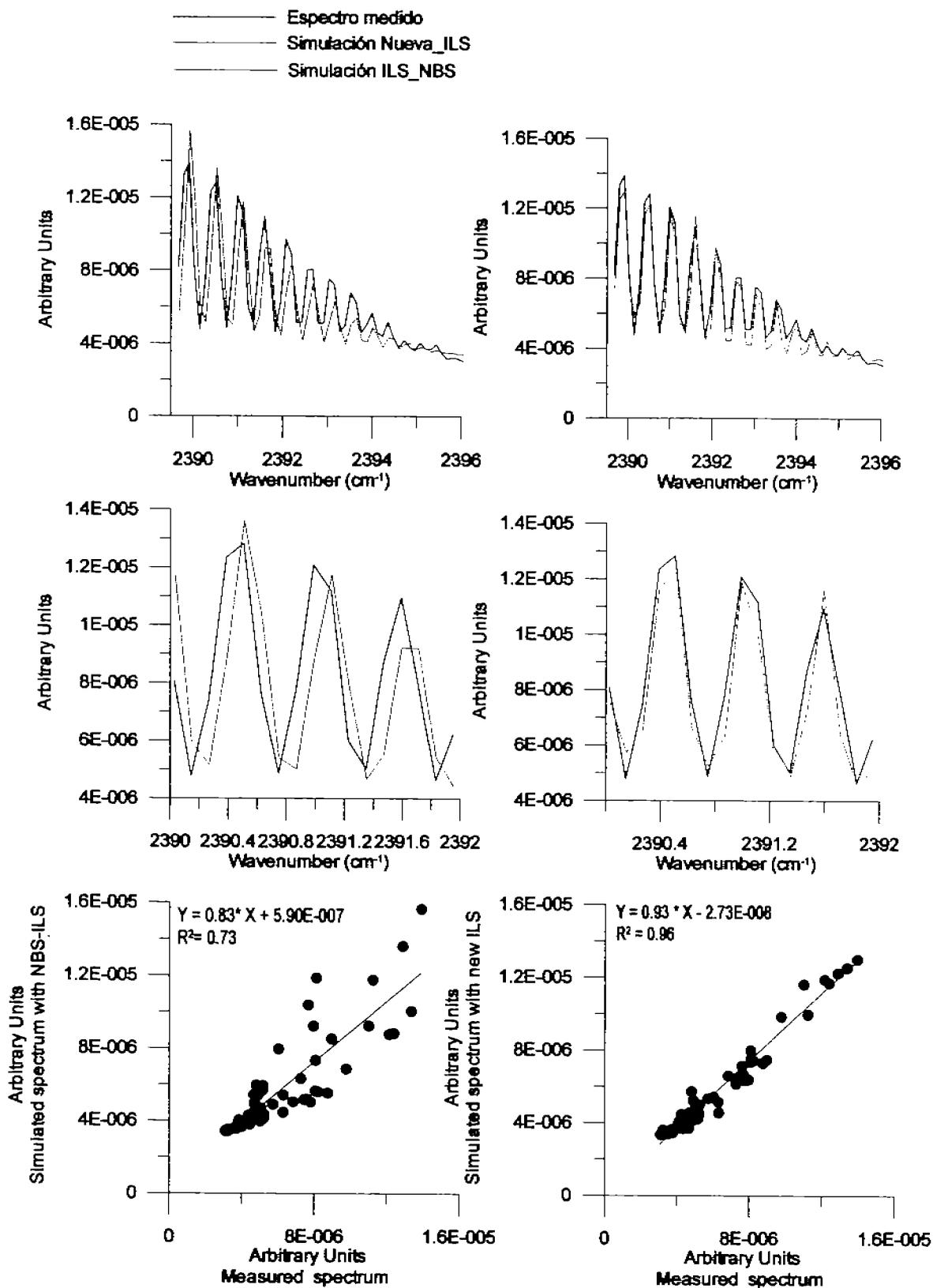


Figure 5: In this figure are shown the simulation of one emission spectrum by MAPS using two different ILS. On the left is shown the NBS ILS simulation, where the correlation factor is 0.68 and on the right the simulation using the calculated OPAG22 ILS with a goodness of fit of 0.94.

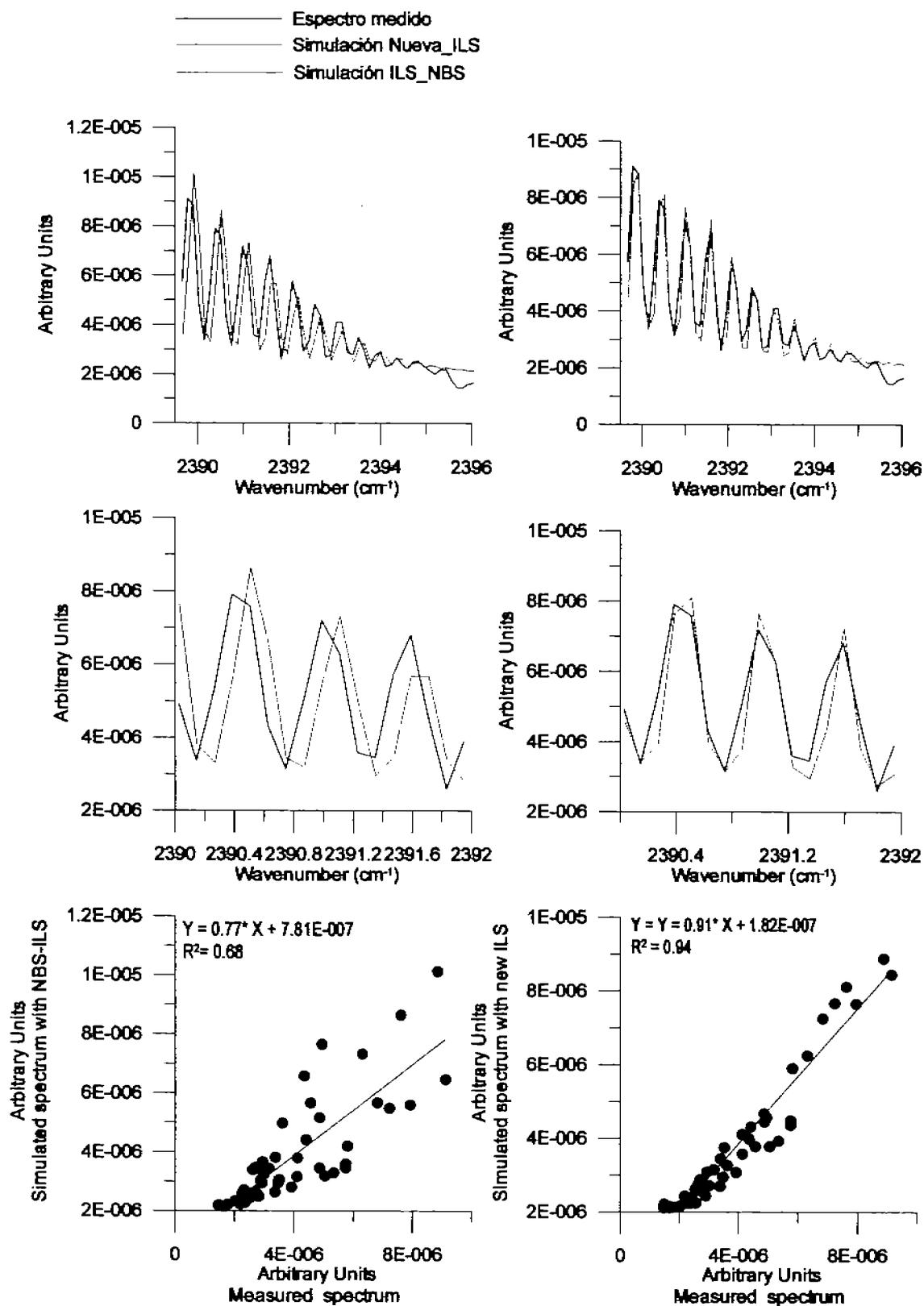


Figure 6: This figure shows the second case of a simulation by MAPS using two different ILS functions. On the left is shown the NBS ILS simulation, where the correlation factor is 0.73 and on the right side the simulation using the calculated OPAG22 ILS with a goodness of fit of 0.96.

3. MEASUREMENT RESULTS

The exhaust of a turbojet based on a Rolls-Royce Gnome 1200, originally operated in a Westland Wessex helicopter, was measured by the SIGIS system. The power turbine and the duct which turns the exhaust 90 degrees in the helicopter installation had been removed from the engine and replaced by a straight jet pipe. Hence, the engine resembled a small turbojet with a higher exhaust temperature and velocity than would be encountered in the standard configuration of a Gnome.

To characterize the exhaust gas, a fast gas temperature scan was performed. As result, an important temperature difference between the upper and lower exhaust area was observed. This temperature difference, by it self represent an interesting result since engine designers can visualize on real time exhaust gas temperature asymmetries present into the engine exhaust plume. Temperature asymmetries that may produce over heating effects on specific exhaust engine components (see Figure 7).

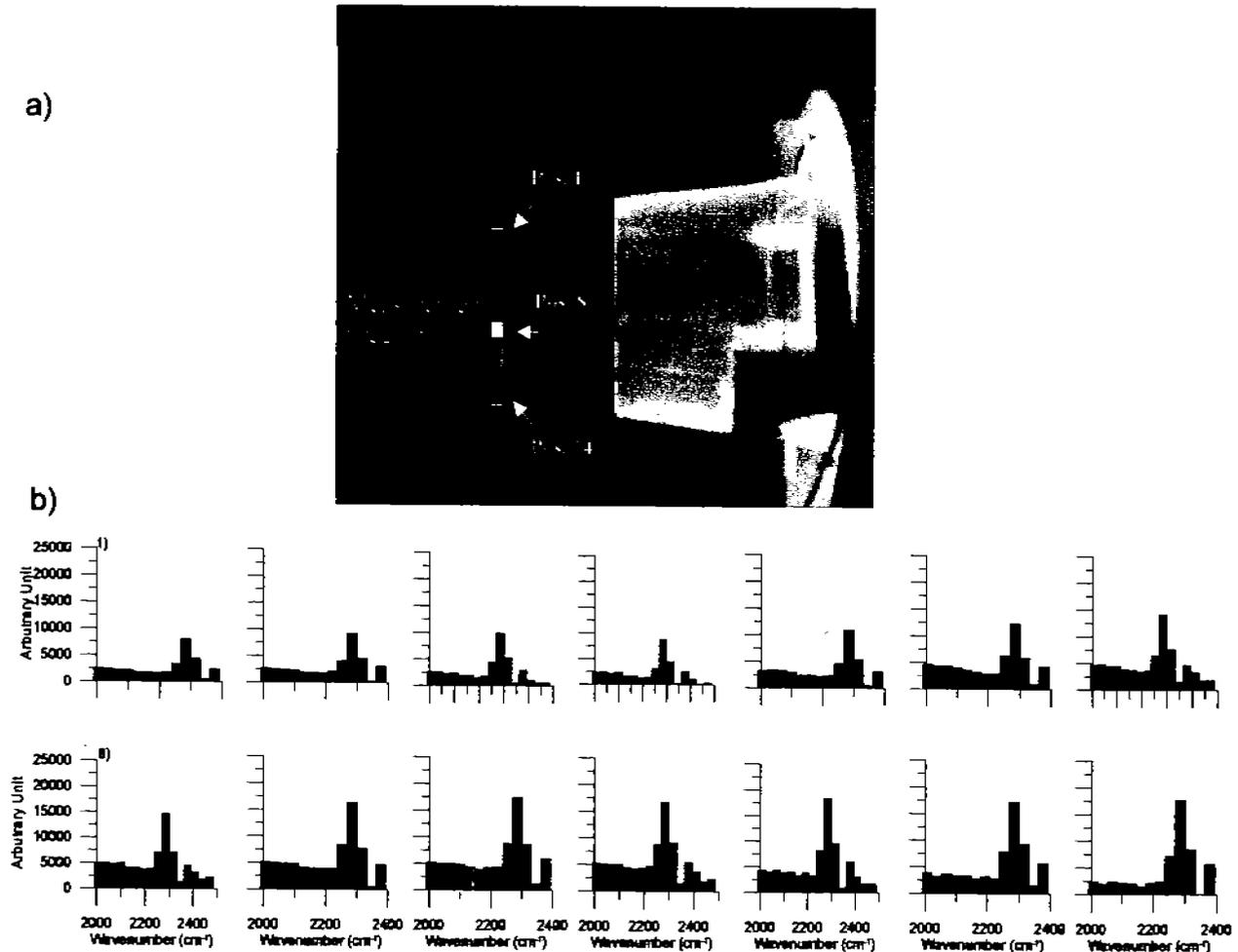


Figure 7: Fast low resolution (0.56 cm^{-1}) scan with automated spectra analysis. a) False colour images generated by fast low resolution scans of the gas temperature distribution of the Gnome 1200 turbine at 19000 RPM. Every scanner-pixel represents a low-resolution spectrum processed by the corresponding evaluation algorithm. The brightness is proportional to the numerical result of the algorithm. The mirror was oriented for recording high-resolution spectra in eight measurement positions. b) Illustration of measured spectra for the algorithm used to evaluate the low-resolution spectra.

The spatial distribution of temperature and combustion gases (NO, CO₂, CO and H₂O) were performed using high-resolution spectra measurements at 0.2 cm⁻¹ in 14 vertical positions. The temperature results were after compared with the local temperature of the engine exhaust measured by a thermocouple installed in the engine (Figure 8).

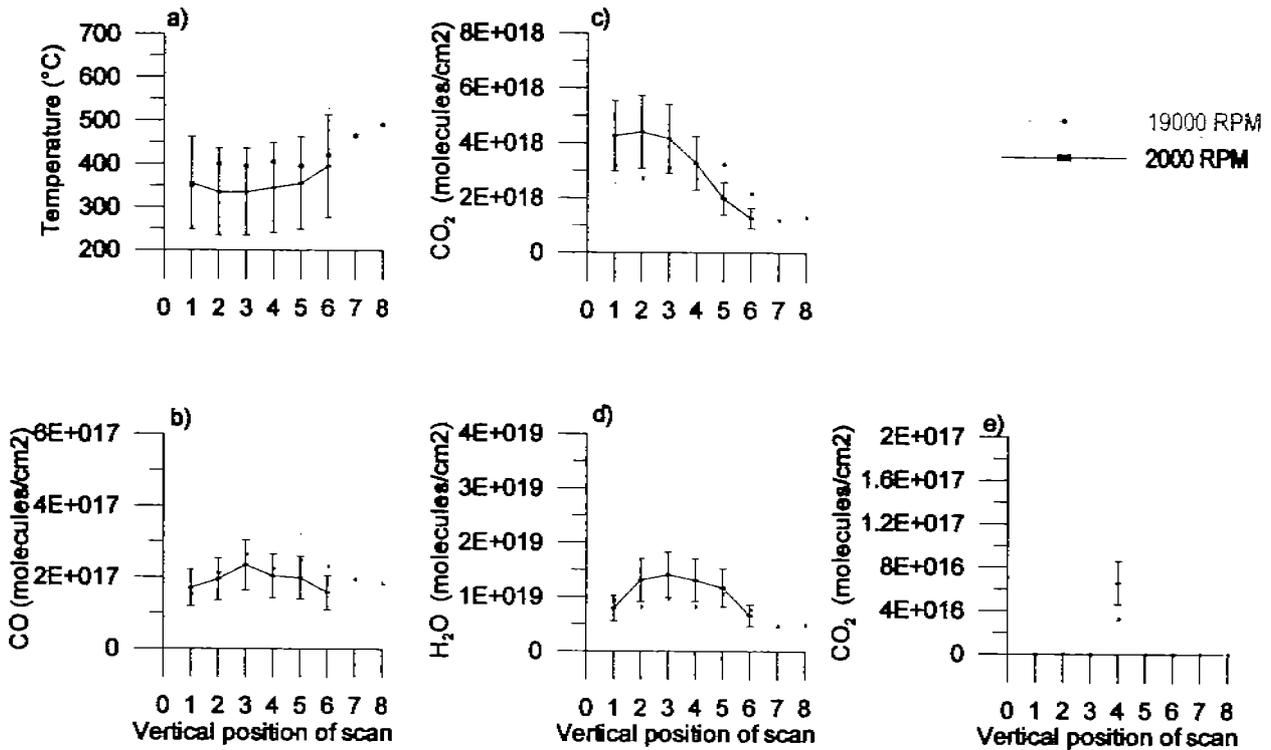


Figure 8: Temperature and CO, CO₂, NO and H₂O vertical profiles of the turbine exhaust at engine speed of 19000 and 20000 RPM. The error bars are $\pm 8^\circ\text{C}$ for the temperature graph and 4% for the concentration.

The average gas temperature calculated by MAPS at the power settings of 19000 and 20000 RPM were $436 \pm 130^\circ\text{C}$ y $353 \pm 106^\circ\text{C}$, respectively. The register temperature by the thermocouple at the same engine power was 430 and 365°C respectively, showing an important agreement between both independent measuring methods.

For CO, the average column density calculated at 19000 RPM was $2.08 \pm 0.62 \times 10^{17} \text{ cm}^{-2}$ and at y 20000 RPM $1.93 \pm 0.57 \times 10^{17} \text{ cm}^{-2}$. The measurement uncertainty of the temperature and concentration calculations was considered as 30% as proposed originally by Heland et al., 1997. The origin of this important uncertainty value is due to the molecular data base uncertainty (HITEMP 15%) and the conversion of the molecular parameters at high temperature.

4. DISCUSSIONS

The calibration method presented in this work allows the determination of the ILS of mobile remote sensing FTIR spectrometry. The method is based on the measurement of the spectrum of a sample gas in a small gas cell at ambient air temperature. Because of this simple setup, the method is applicable on-site. A well characterized ILS is a prerequisite for accurate results of retrieval algorithms. The presented model and the ILS determined by the method described allow the characterization of the ILS even if the instrument is not perfectly aligned or the ILS is degraded by aberrations. By including the real ILS of the spectrometer OPAG22 it was possible to improve substantially (from -0.7 to 0.9) the correlation between measured and the calculated spectra.

In the Gnome test bed measurements was observed that the system allowed the detection of important differences in temperature and concentration in dependence from the engine operation and in the case of temperature measurements the calculated temperature results were consistent in all cases with the temperature an independent method.

5. CONCLUSIONS

Scanning imaging FTIR emission spectrometry allows characterizing the spatial distribution of exhaust gas as well as quantifying the emissions of aircraft. The system SIGIS-HR in combination with the new version of the software MAPS allows measurements in test beds. Among the advantages of performing measurements as described in comparison to the standard methods are:

- An excellent exhaust plume visualization that makes it possible for the operator to localize within a few seconds the exhaust plume.
- Easier high resolution spectra recorded by improvements in the localization and detection of infrared radiation.
- Possibilities to perform a thermo-scan that shows radiation temperature distribution anomalies of hot gas within the engine exhaust.
- No evidences of noise disturbance on the spectra during test bed and at airport measurements.

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Remote Sensing of aircraft emissions by scanning imaging FTIR spectrometry

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ABSTRACT

The Scanning Infrared Gas Imaging System (SIGIS) was used to perform non intrusive measurements of a Boeing 737 and a diesel powered burner (used as a hot gas producer). During the measurements it was observed that the selection of the optimal measurement positions into the plume, visualised by an infrared image from a real-time infrared camera in which the emission intensity of different field of view (FOV) positions into the plume are plotted in false colours, is possible very precisely. This enhanced considerably the probability of detection of infrared radiation emitted by a hot gas plume (e. g. from an in-service aircraft at the ground) for the objective to determine composition and temperature of the exhausts. Using this improved localization of the optimum measurement position into the hot exhaust plume the temperature and the concentrations of CO, CO₂ and NO were calculated. Additionally, the spatial distribution of gas temperature and concentrations of CO, CO₂ and NO into the exhaust plume were determined.

Keywords: non-intrusive measurement techniques, FTIR, IR camera, imaging spectrometry, aircraft exhausts

1. INTRODUCTION

The potential environmental impact of aircraft emissions and economical aspects require that engine manufacturers develop engines with lower trace gas and particle emissions, but at the same time with high efficiencies. Each new engine developed must be shown to meet the environmental requirements laid down by regulatory bodies, thus the exhaust gas measurements which accompany all stages of engine development are an essential part of this process. Within this framework, engine manufacturers stress the necessity of implementing new methodologies capable of measuring in real time key components of the engine exhaust (CO₂, CO, H₂O, NO and NO₂) which are highly dependant on the engine's operations. The existing methodology to measure the composition of aircraft exhaust is based in exhaust gas sampling by rake probes that are followed by heated transfer lines which transport the sample gas into different measurement instruments (Ref ICAO).

During the last few years studies using passive Fourier Transform Infrared (FTIR) spectrometry measuring aircraft engine emissions, in test beds (Schäfer et al., 2000)¹ and on in-service aircraft at airports (Heland, Schäfer, 1997²; Heland, Schäfer, 1998³; Schäfer et al., 2003⁴), have shown that this technique offers important advantages, when compared to conventional measurement methods. The conventional International Civil Aviation Organization regulated methods (ICAO, 1993)⁵ involve exhaust gas sampling by a rake of probes, followed by transfer of the sample in heated lines to different instruments for analysis of various molecular pollutants: non-dispersive infrared detectors for CO and CO₂, chemiluminescence analysers for NO_x and flame ionisation detectors for unburnt hydrocarbon (UHC)., FTIR advantages include:

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- low operational costs,
- ease of handling,
- online measurements,
- possibility of re-analysis without affecting the data source (measured spectra),
- no extractive sampling, thus avoiding any chemical changes which may occur within the probe and extraction system before reaching analytical equipment,
- reduced risk of engine damage,
- possibility to perform measurements of aircraft engines during real airport operations.

Remote sensing by passive FTIR spectrometry allows the retrieval of column densities or concentrations of molecules in gas plumes such as exhaust plumes of aircraft, smoke stacks and flares or vapor plumes emitted after chemical accidents (Grant et al., 1992⁶; Haus et al., 1994⁷; Lindermeir, 1994⁸; Haus et al., 1998⁹; Hilton et al., 1998¹⁰; Schäfer et al., 2004¹¹). Different FTIR spectrometers e.g. the high-resolution spectrometer K300 (Haus, et al., 1994)⁷ (Kayser-Threde GmbH, Munich, Germany) and the scanning imaging spectrometer SIGIS-HR (Harig, Matz, 2001¹²; Rusch et al., 2005¹³) were used for measurements together with the lineby-line spectra retrieval software MAPS (Haus et al., 1994⁷; Heland, Schäfer, 1997²; Flores-Jardines et al., 2005¹⁴). For calibration of the measurement results the real instrumental line shape function (ILS) is determined. This procedure offers the possibility to check correct optical alignment of the spectrometer which cannot be tested by radiometric calibration and signal check, but which can cause errors in concentration retrieved from spectra. A method is developed for determination of instrument performance specifications for all modes of FTIR spectrometry on the basis of determination of ILS as described by Harig (2004)¹⁵. This quality assurance / quality control (QA/QC) method for passive and active non-intrusive instrumentation on the basis of FTIR spectrometry is applied (Harig et al., 2005)¹⁶. The procedure was tested on a small turbojet engine on a test bed run under different engine conditions.

The measurement method and the results of the investigations of the temperature and gas concentrations (CO, NO) within the aircraft engine plume are described in the following.

2. EXPERIMENTAL SET-UP

Figure 1 shows the experimental set-up for the aircraft exhaust measurements during the Budapest airport campaign in October 2004. The SIGIS HR system was pointed behind the engine and the APU exhaust during the taxi way and the parking place respectively. Instead to adjust the telescope to receive the maximum signal manually (as in previous measuring campaigns), a fast temperature scan was performed by the SIGIS HR system to visualise the plume shape characteristics and to localise the position where the signal was a maximum inside a pre-selected area. This procedure reduced the time to set the measuring position to a few seconds and enhanced the probability of detection from the infrared radiation emitted by the hot exhaust plume. After the measuring position was established, a high resolution spectrum at 0.2cm^{-1} was recorded.

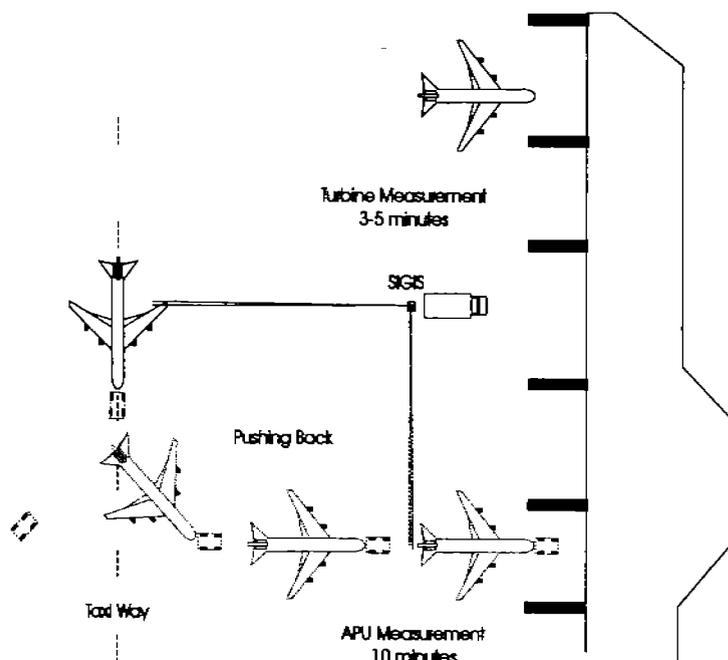


Figure 1: Scheme of the experimental set-up for measuring aircraft exhaust emissions with the SIGIS HR system at high spectral resolution. The measuring position shown allows for investigation of the aircraft situated at a parking position and on the taxiway.

3. INSTRUMENTATION

The SIGIS HR system is able to visualise the spatial distribution of the temperature of the plume by performing a two dimensional scan at different spectral resolutions. It is comprised of an OPAG 22 interferometer (Bruker) with an operating range between 680 and 6000 cm^{-1} (MCT detector) and a maximum spectral resolution of 0.2 cm^{-1} , an azimuth-elevation-scanning mirror actuated by stepper motors, a data processing and control system with a digital signal processor (FTIR DSP), and an image processing system (Video DSP). An IR camera coupled with the Video DSP completes the system. A full description of the instrument and its characteristics has been presented elsewhere^{6,7}. In Figure 2 an example of an aircraft measurement scheme by the SIGIS HR system at the taxiway is shown.

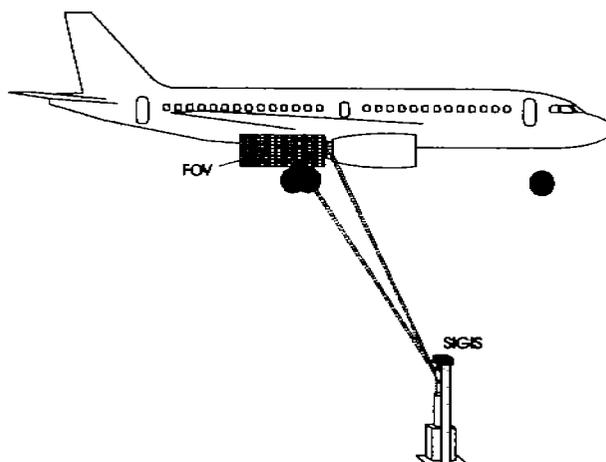


Figure 2. Example of an aircraft measurement scheme by the SIGIS HR system at the taxiway. The black rectangle corresponds to the scanned area focused by the field-of-view (FOV) from the spectrometer.

4. THE RADIATIVE TRANSFER MODEL

Basically, the propagation of monochromatic infrared radiation coming from a hot exhaust plume in the atmosphere is described by the following expression (details are in⁸):

$$\frac{dI_{\sigma}}{ds} = -\beta I_{\sigma} + \beta J_{\sigma} \quad (1)$$

where I_{σ} is the intensity of radiation and β is the volume extinction coefficient that includes the contribution of the individual lines of a chemical species, is valid for monochromatic radiation and consists of two terms, the extinction represented by $-\beta I_{\sigma}$ and the emission represented by $+\beta J_{\sigma}$. For this model, the atmosphere is divided into discrete homogeneous layers in which local thermodynamic equilibrium can be assumed.

Deriving the transmission expression $\tau = \exp^{-\tau(x)}$, and introducing this in the equation (1), we can obtain the radiation that reaches the spectrometer interpreted as:

$$I_{\sigma}(2) = I_{\sigma}(1)\tau + \int_{\tau(1)}^1 J_{\sigma} d\tau \quad (2)$$

and for m th layers application:

$$I_{\sigma} = \tau_m I_{\sigma, m-1} + (1 - \tau_m) J_{\sigma}(T_m) \quad (3)$$

where $\tau_m I_{\sigma, m-1}$ represent the absorption term and $(1 - \tau_m) J_{\sigma}(T_m)$ the self radiation term of the m th layer².

4.1 Line-by-line procedure

In principle, the interpretation of the recorded spectra is done by calculating synthetic spectra at different temperatures and concentrations and then comparing them with the measured spectra by the least-squares-fitting technique. To simulate synthetic spectra, a radiative transfer model is used to describe the radiation transport of the incoming infrared radiation from a hot source into the atmosphere. The Multi-component Air Pollution Software (MAPS) is used to interpret the spectrum recorded during the measurements and is based upon line-by-line calculations of the thermal emission and molecular absorptions of the air components⁹.

As a first step, a quantitative analyses of the CO₂ emission spectrum is performed in the spectral window 2387 - 2397 cm⁻¹ by simulating line-by-line 19 individual transitions at different temperatures and concentrations (see Figure 3) using the molecular parameters extracted from the HITRAN data base^{10, 11}. Since the overall intensity of this region is dependent upon the temperature and concentration, the measured radiance is compared with the synthetic spectra, as described above, in order to provide the optimal data set.

As a second step, and with the knowledge of the plume's temperature, the concentrations in the lines around 2099 cm⁻¹ and 2169.2 cm⁻¹ are calculated for H₂O and CO, respectively. For the NO concentration evaluated at 1900.3 cm⁻¹, pre-calculated concentrations of H₂O and N₂O (at 2190 cm⁻¹) are used in the least squares procedure¹².

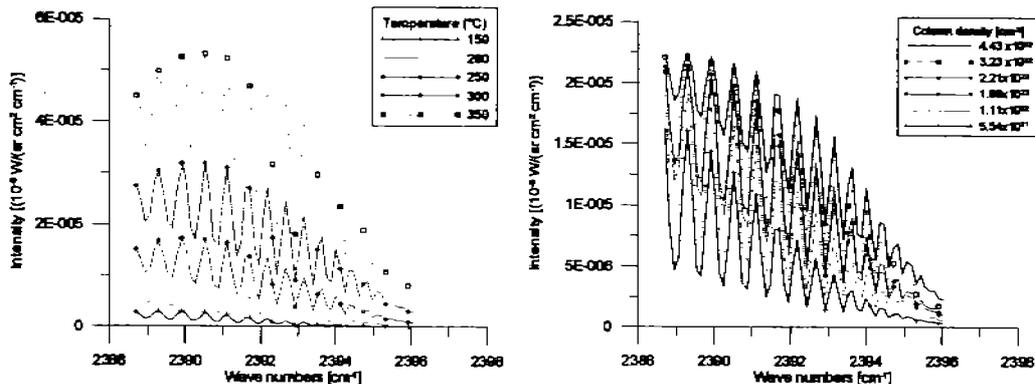


Figure 3. High resolution synthetic spectra of the CO₂ region by MAPS at six different temperature and column density levels.

The emission index of a species X is then calculated based on the equation

$$EI(X) = EI(CO_2) \times \frac{M(X)}{MI(CO_2)} \times \frac{Q(X)}{Q(CO_2)} \quad (4)$$

where *M* denotes the molecular weight and *Q* the concentrations (mixing ratios, column densities, etc.) of the species and *EI(CO₂)* is known from stoichiometric combustion as 3,150 g/kg.

5. EXPERIMENT

5.1 Aircraft measurements

Measurements of the CFM56-7B24 engine (Figure 4a) and the Auxiliary Power Unit (APU) of a Boeing B737 aircraft were obtained by SIGIS system (Figure 4b).

The spectra from the APU and the turbines were recorded at high resolution (0.2 cm⁻¹) from a 40 and 80 m distance, respectively. The positions of the field-of-view (FOV) were selected by scanning within the area where the plume was expected, as shown in the rectangles of Figure 4. After simulating the infrared incoming radiation, the retrieved temperatures for the APU unit and the turbine were 290 and 390°C, respectively. Figure 5 shows the comparison of the simulated emission spectra from CO₂ at different temperatures and column densities.

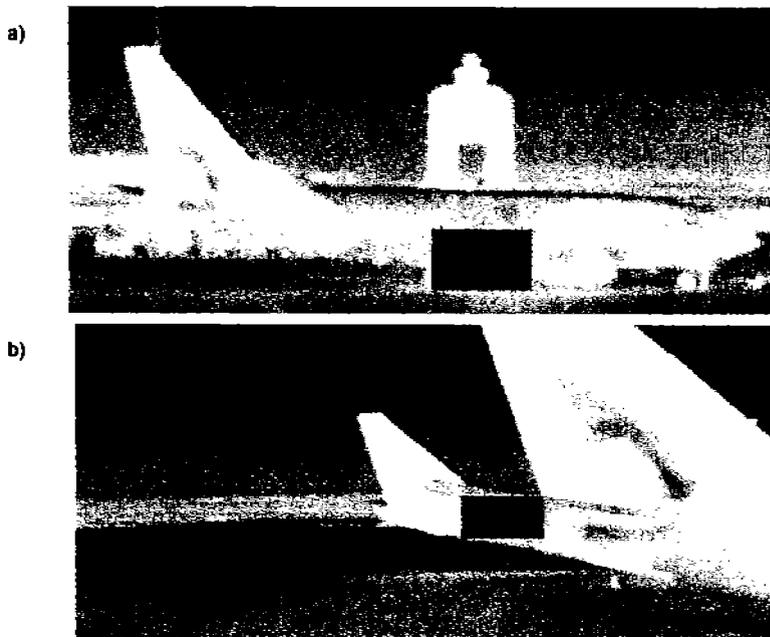


Figure 4. Thermal images by an IR camera from a CFM56-7B24 engine (a) and an APU (b) from a B737-7Q8. The measuring position of the high resolution spectra is shown and the fast temperature scan of the turbine is represented by false colour.

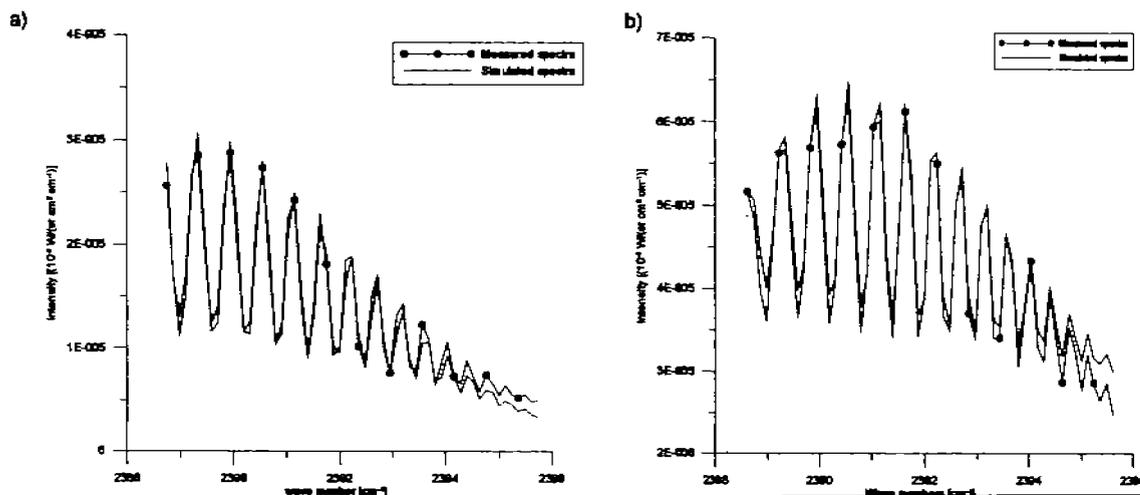


Figure 5. Comparison of two high resolution spectra measured from an APU (a) and a turbine type CFM56-7B24 (b) from two B737-7Q8 aircrafts and the simulated spectra from MAPS.

The calculated emission indices from the APU and the turbine type CFM56-7B24 taken as the average of 3 observations are listed in the tables 1 and 2 (together with ICAO data). In Figure 6 and 7 the measured NO and CO emission spectra are shown, respectively.

Table 1. Emission indices of the Auxiliary Power Unit (APU) from the B737-7Q8.

Compound	Calculated Emission Index
CO	22 (g/kg)
NO	0.20 (g/kg)

Table 2. Emission indices from the CFM56-7B24 engine type from the B737-7Q8 together with ICAO data⁵.

Compound	Calculated Emission Index	ICAO
CO	29 (g/kg)	22 (g/kg)
NO	4.21 (g/kg)	4.4 (g/kg)

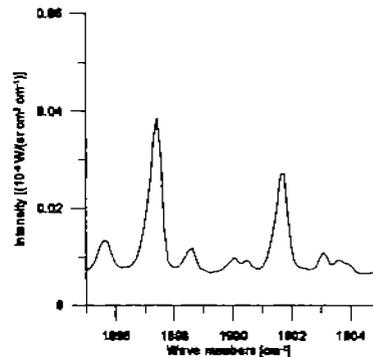


Figure 6. NO emission spectra of the turbine type CFM56-7B24 (B737) measured by the SIGIS HR system.

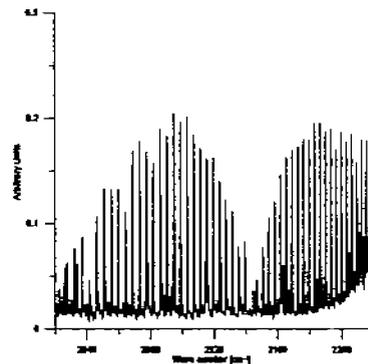


Figure 7. CO emission spectra measured by the SIGIS HR system from the turbine type CFM56-7B24 (B737).

5.2 Experimental set-up for the high temperature exhaust producer

With the objective to show the detection possibilities of NO emissions, a second experiment using a diesel powered burner was performed with the SIGIS HR system. A schematic drawing of the diesel powered burner is shown in Figure 8. The inner diameter of the steel burner tube is 50 cm and its length is 120 cm. The distance of the burner axis to the ground is about 120 cm. The burner, using diesel as fuel, has a maximum power of 356 kW. The airflow inside the tube is 40,000 l/min¹³.

The SIGIS HR system spectrometer was placed 9.5 meters away from the burner and its telescopic mount was orientated towards the exhaust stream directly behind the burner nozzle exit. Initially, the spatial temperature distribution of the nozzle area was fast-scanned at low resolution (56 cm⁻¹) with the SIGIS HR system integrated to the spectrometer to select a high resolution spectra record position.

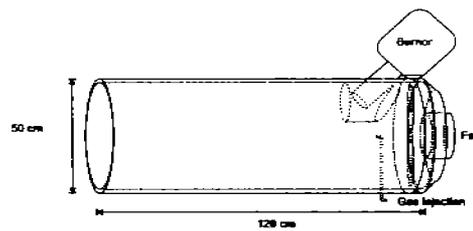


Figure 8: Sketch of the construction and dimensions of the powered diesel burner.

5.2.1 Temperature distribution

The first measurement of the plume stream was performed by a fast temperature scan which plots the temperature distribution. Figure 9 shows the scanned field of view within the plume, it is important to observe the colour contrast between different pixel positions produced principally by non homogeneous gas distribution of the hot exhaust. To quantify the intensity of the temperature gradient in a selected area of the hot stream, the plume was divided into small homogeneous segments. Two pixel positions separated by ~ 10 cm were selected to record two high resolution spectra (0.2 cm^{-1}). After quantitative analysis of the observed spectra, the temperature difference between both positions was found to be $320 \text{ }^\circ\text{C}$ and the radiation measured in the hot stream from this device was highly dependent on the relative measuring position due the non homogeneous gas distribution.

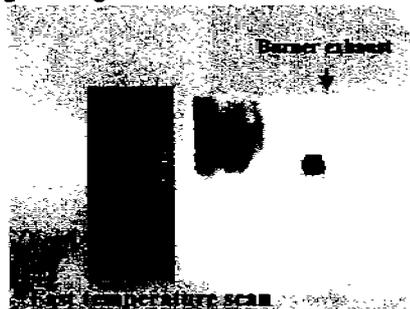


Figure 9: Infrared camera image overlapped with a low resolution scan (56 cm^{-1}) for fast temperature gas identification of the diesel powered burner from a fixed position measurement.

5.2.2 Gas concentration profile

To characterise the homogeneity of the exhaust plume¹⁴, vertical measurements were recorded from the diesel powered burner. From the quantitative gas analysis described before, the temperature and concentrations profile were obtained and are presented in Figure 10. It is possible to observe an important asymmetry between the temperature and gas concentration profiles in the hot exhaust plume.

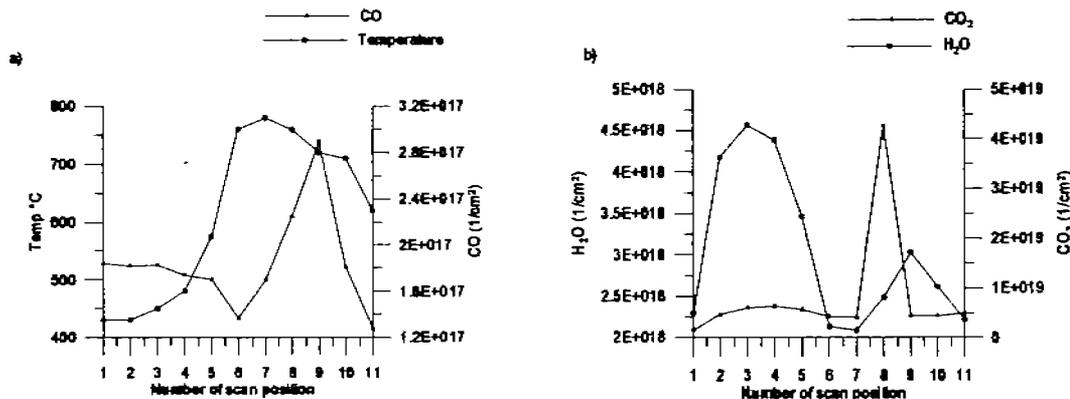


Figure 10: Spatial distribution of temperature and gas concentration of CO a) and CO₂ and H₂O b) calculated in the hot exhaust plume.

5.2.3 NO injection

Due to the low emission rate of NO gas from the diesel powered burner (lower than the detection limit), 10 l/min of pure NO was injected into this device and high resolution spectra were recorded. Different horizontal downstream positions were located using the FOV of the spectrometer by the SIGIS HR system (see Figure 11).

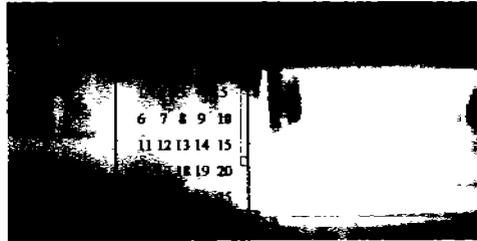


Figure 11: Infrared image of the diesel powered burner recorded during the downstream measurements. The area in the box represents the high resolution spectra record positions during the measurement.

The resultant spectrum of the measurements gave a high intensity NO signal, from which it was possible to observe differences in the NO emission lines in the recorded spectra at different field of view positions (see figure 12).

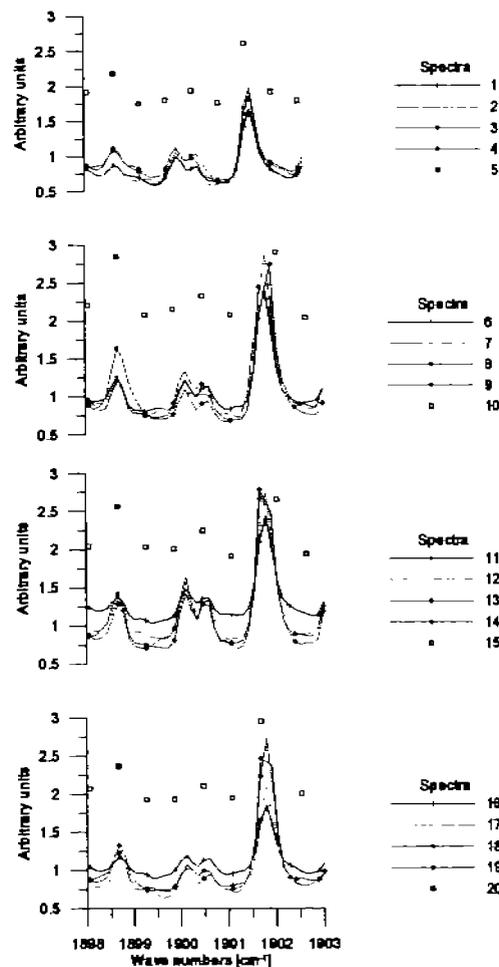


Figure 12: High spectra resolution recorded at twenty different plume positions from the diesel powered burner.

After the quantitative analysis of every recorded spectrum, a temperature profile downstream from the hot exhaust plume was calculated and plotted (see Figure 13). The downstream temperature profile shows a high asymmetry in the exhaust gas temperature.

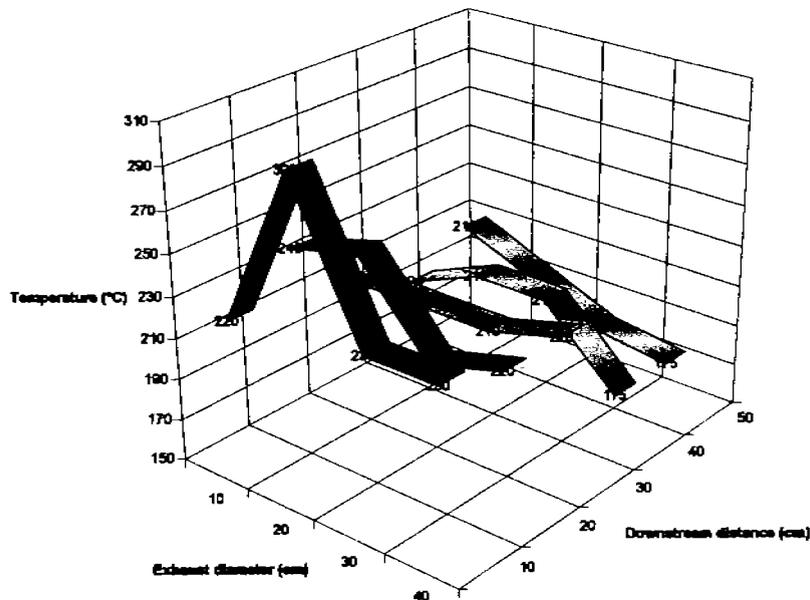


Figure 13: Temperature spatial distribution of the hot gas exhaust at four horizontal and five downstream positions.

Using the infrared image recorded from the hot gas exhaust during the non-intrusive measurements, different zones were identified within the burner exhaust where the mass transfer from the hot gas stream was influenced by different effects (Figure 14).

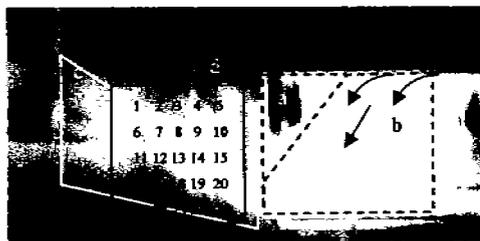
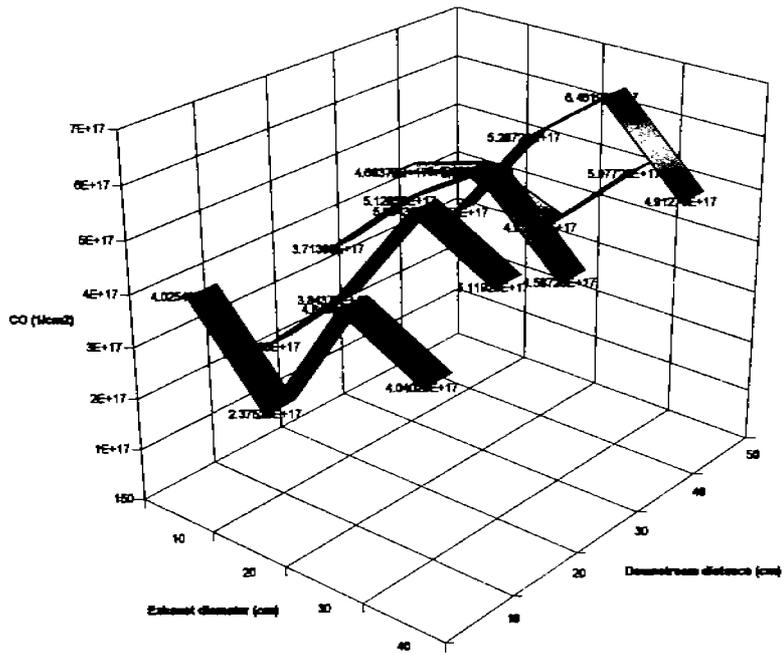


Figure 14: Infrared image from the diesel powered burner. The Figure shows the flux behaviour of the burner powered by diesel in four sections, a) represents a relative colder zone in the exhaust tube where the gas transport is relatively low, b) represents the exhaust area where the hot gas stream impact the tube producing a cyclone flux, c) represents the area where the main gas stream is present and d) the zone where are present import gas vortex.

Figure 15 presents the CO and NO exhaust distribution. In the NO spatial distribution graph it is possible to observe an important inconsistency in the NO emitted rate. The NO column density is growing downstream, but in theory the NO should be lower downstream due to the dilution and reaction with the O₂ within the plume. The reason for this effect is that gas streams coming from the very lower exhaust parts are not included in the measurements directly behind the burner exit. These streams are carrying the injected NO and are going up downstream.

a)



b)

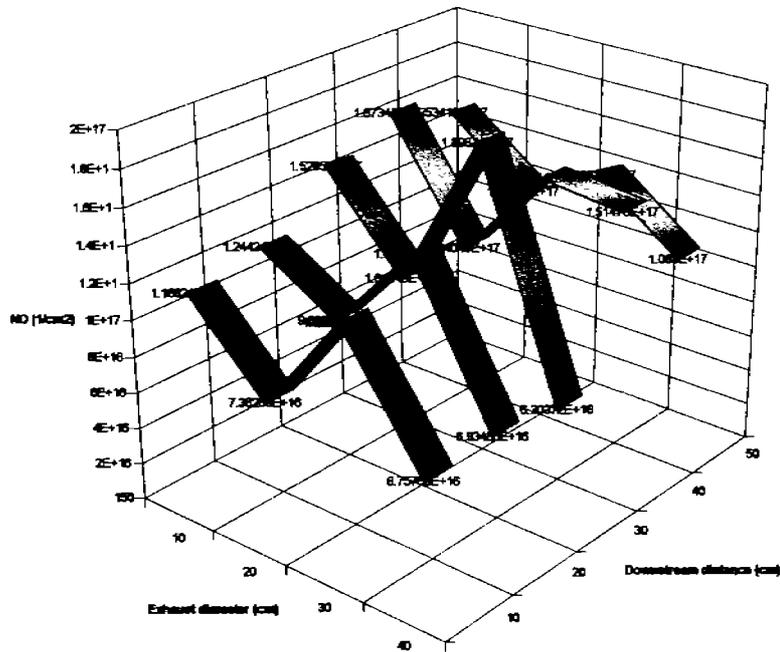


Figure 15: CO (a) and NO (b) spatial distribution of the hot gas exhaust at four horizontal and five downstream positions.

6. CONCLUSIONS

It has been observed that the SIGIS HR system enhances the probability of emissions detection, providing an important tool in the field of the FTIR emission spectroscopy.

A. Aircraft exhaust measurements

The exhaust composition obtained from the aircraft measurements of the turbine type CFM56-7B24 (B737) presented an increase with respect to the emission index reported by ICAO of 31% for CO. This difference has been also observed into the emission indices reported for different engine aircrafts in previous investigations⁴. These results show that the measurements done with the SIGIS HR system and the analytical software MAPS for in-work aircraft conditions can be highly reliable and the technique is enhanced.

B. Hot exhaust producer measurements

Although the emission indices given by our hot gas producer presented low reproducibility due to the technical characteristics of our device, a hot gas stream was obtained in which it was possible to inject pure NO and CO in different flux rates. All this effort had as objective to observe the operation ability of the SIGIS HR system and the analytical software MAPS to obtain detailed information from different segments inside the hot exhaust plume.

The emission spectra after scanning 11 vertical positions inside the hot exhaust plume showed well defined and strong CO spectra intensity for every one of the measure positions. This gave as result a particular vertical profile of temperature that had as characteristics a non-homogeneous spatial distribution. Also from the downstream scan in 4 horizontal levels after injection of pure NO (10 l/min) a high intensity NO signal was observed into the resultant spectrum where important differences in the NO emission lines from the recorded spectra at different measurement positions were present. This enabled the production of a downstream profile of NO of the hot exhaust plume. This was also done for temperature and CO concentration.

For all these results the application of the SIGIS HR system and the software MAPS showed the advantages and disadvantages of a hot exhaust producer and the possibilities for evaluation of plume models (see also¹²).

7. ACKNOWLEDGEMENTS

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Remote sensing of aircraft exhaust temperature and composition by passive Fourier Transform Infrared (FTIR)

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ABSTRACT

The scanning infrared gas imaging system (SIGIS-HR) and the quantitative gas analysis software MAPS (Multicomponent Air Pollution Software) are applied to investigate the spatial distribution of the temperature and gas concentrations (CO, NO) within the plume of aircraft engines at airports. The system integrates an infrared camera also. It is used for the localisation of the hot source that additionally suggests the best measurement position of the SIGIS-HR. The application of emission FTIR spectrometry for the measurement of temperature and gas emission index of CO and NO is presented for the exhaust of a small turbojet based on a helicopter turbine. In these measurements the emitted infrared radiation from the exhaust gas stream was collected by the SIGIS-HR at different spectral resolution (56 cm^{-1} and 0.2 cm^{-1}). The software MAPS includes the Instrumental Line Shape (ILS) of the OPAG- 22 FTIR spectrometer obtained by active gas cell measurements and ILS modelling.

The rough concept of the system will be presented and operational applications will be discussed. The results of the investigation of the temperature and gas concentrations (CO, NO) within the aircraft engine plumes will be shown. The limitations and of the systems will be discussed.

Keywords: Air pollution, passive FTIR, aircraft emissions, airport emissions.

1. INTRODUCTION

During the last few years studies using passive Fourier Transform Infrared (FTIR) spectrometry measuring aircraft engine emissions, in test beds (Schäfer et al., 2000)¹ and on in-service aircraft at airports (Heland, Schäfer, 1997²; Heland, Schäfer, 1998³; Schäfer et al., 2003⁴), have shown that this technique offers important advantages, when compared to conventional measurement methods. The conventional International Civil Aviation Organization regulated methods (ICAO, 1993)⁵ involve exhaust gas sampling by a rake of probes, followed by transfer of the sample in heated lines to different instruments for analysis of various molecular pollutants: non-dispersive infrared detectors for CO and CO₂, chemiluminescence analysers for NO_x and flame ionisation detectors for unburnt hydrocarbon (UHC). FTIR advantages include:

- low operational costs,
- ease of handling,
- online measurements,
- possibility of re-analysis without affecting the data source (measured spectra),

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- no extractive sampling, thus avoiding any chemical changes which may occur within the probe and extraction system before reaching analytical equipment,
- reduced risk of engine damage,
- possibility to perform measurements of aircraft engines during real airport operations.

Non-intrusive techniques capable of measuring in real time key components of the engine exhaust (CO_2 , CO , H_2O , NO and NO_2) which are highly dependent on the engine's operations would be extremely useful to engine manufacturers. .

Remote sensing by passive FTIR spectrometry allows the retrieval of column densities or concentrations of molecules in gas plumes such as exhaust plumes of aircraft, smoke stacks and flares or vapor plumes emitted after chemical accidents (Grant et al., 1992⁶; Haus et al., 1994⁷; Lindermeir, 1994⁸; Haus et al., 1998⁹; Hilton et al., 1998¹⁰; Schäfer et al., 2004¹¹). IR radiation emitted by exhausts or gas plumes is detected. Different FTIR spectrometers e.g. the high-resolution spectrometer K300 (Haus, et al., 1994)⁷ (Kayser-Threde GmbH, Munich, Germany) and the scanning imaging spectrometer SIGIS-HR (Harig, Matz, 2001¹²; Rusch et al., 2005¹³) were used for measurements together with the line-by-line spectra retrieval software MAPS (Haus et al., 1994⁷; Heland, Schäfer, 1997²; Flores-Jardines et al., 2005¹⁴). For calibration of the measurement results the real instrumental line shape function (ILS) is determined. This procedure offers the possibility to check correct optical alignment of the spectrometer which cannot be tested by radiometric calibration and signal check, but which can cause errors in concentration retrieved from spectra. . A method is developed for determination of instrument performance specifications for all modes of FTIR spectrometry on the basis of determination of ILS as described by Harig (2004)¹⁵. This quality assurance / quality control (QA/QC) method for passive and active non-intrusive instrumentation on the basis of FTIR spectrometry is applied (Harig et al., 2005)¹⁶. The procedure was tested on a small turbojet engine on a test bed run under different engine conditions.

The measurement method and the results of the investigations of the temperature and gas concentrations (CO , NO) within the aircraft engine plume are described in the following.

2. METHODOLOGY

2.1 Radiative transfer models

State-of-the-art quantitative retrieval algorithms of passive remote sensing by FTIR spectrometry (Goody, Yung, 1989¹⁷; Haus et al., 1994⁷; Harig, 2004¹⁵) require two models: a radiative transfer model and an instrument line shape model, the ILS. The real ILS of FTIR spectrometers differs significantly from ideal, particularly if the instrument is optimized for high signal-to-noise ratio, which is achieved by interferometer designs with high optical throughput (étendue). The real ILS may be modelled by convolution of the ILS of the ideal FTS with a so-called inherent ILS describing the deviations. In this work, the inherent ILS is modelled by a function which is dependent on a small number of parameters (Harig et al., 2005)¹⁶.

The possibility of a frequent determination of the ILS is advantageous especially in the case of mobile spectrometers because the alignment of the interferometer may be altered by the transport of the system. In addition to the provision of the actual ILS at the time of the measurement for the retrieval algorithm, an on-site determination of the ILS is a functional test of the spectrometer. A potential degradation of the quality of the spectra may be identified quickly and measures to improve the quality may be taken immediately. However, even if it is not possible to remove the cause of a degraded ILS on site, an accurately determined ILS may be used for the quantitative analysis of the spectra.

The basic characteristics of spectra measured by a passive FTIR spectrometer may be described by a model in which the atmosphere is divided into plane-parallel homogeneous layers along the optical path (Beer, 1992)¹⁸. In many cases a model with three layers is sufficient. Radiation from the background, for example the sky or a surface (background layer), propagates through the plume (cloud or plume layer, a mixture of the plume molecules and air), and the atmosphere between the plume and the spectrometer (atmospheric layer). The radiation containing the signatures of all layers is measured by the spectrometer. The plume layer and the atmospheric layer are considered homogeneous with regard to all physical and chemical properties. Because the scattering coefficient in the infrared spectral region is small under many measurement conditions, the contribution of scattering is neglected in this model. If the assumption of three

homogeneous layers is not warranted, for example if there are strong temperature gradients within the layers, additional layers may be added (Haus et al., 1994⁷; Heland, Schäfer, 1997²; Heland, Schäfer, 1998³; Schäfer et al., 2000¹).

For an ideal interferometer operating with perfectly collimated radiation, the ILS is given either by the Fourier transform of the function describing the finite movement of the mirror or the Fourier transform of the apodization function. In practice, in particular in the case of a passive remote sensing interferometer optimized for high throughput, non-paraxial rays from a finite source reach the detector causing a broader ILS and a frequency shift. In this case, the ILS is given by the convolution of the Fourier transform of the function describing the finite movement of the mirror and the inherent apparatus function (Beer, 1992)¹⁸, which is a function describing the effect of broadening and the frequency shift. In the case of a homogeneous source and an ideal Michelson interferometer (ideal mirrors etc.), in which the radiation leaving the interferometer is measured by a detector in the focal plane of a condenser lens (or mirror), the inherent apparatus function is a rectangular function (boxcar). In a small spectral range the spectrum may be approximated by a convolution of the true spectrum with the apparatus function. In order to characterize the combined effects of aberrations, misalignment, nonlinear movement of the mirrors etc., empirical apparatus functions may be used. For passive remote sensing FTIR spectrometer measurements this has been described in Harig (2004)¹⁵. For the determination of the ILS, i.e. for modelling of measured spectra, an ILS function calculated using an empirical inherent apparatus function defined by five parameters is used. This model contains the inherent apparatus function of the ideal Michelson interferometer illuminated by an extended homogeneous source as a limiting case and it contains an approximation for the inherent apparatus function of the interferometer without collimator and condenser.

2.2 Method for the Determination of the Instrument Line Shape

In order to determine the ILS, a spectrum of a well-known gas sample contained in a gas cell is measured (Harig et al., 2005)¹⁶. The radiation source is a black body. The determination of the ILS is performed by minimization of the difference between the measured spectrum and a spectrum calculated using a model. The model contains two sub-models, a radiative transfer model for the radiance at the entrance aperture of the interferometer and a model describing ILS. A measured high-resolution spectrum is used for this method. In order to minimize computation time, the (apparent) transmittance of the gas layer is approximated by convolution of a spectrum of the calculated transmittance (monochromatic) with the normalized ILS. The background layer is modelled using the spectral resolution of the measurement. In the case of a slowly varying background radiance, this method yields a good approximation in a small spectral range. The best-fit parameters are determined by the Levenberg-Marquardt method. In order to quantify unknown samples, an analogous method with fixed ILS parameters is applied.

2.3 Instrumentation

All measurements were performed with the scanning infrared gas imaging system SIGIS-HR. The SIGIS-HR is comprised of an interferometer (OPAG 22, Bruker Daltonik, Leipzig, Germany), a telescope, an azimuth-elevation-scanning mirror actuated by stepper motors, an infrared camera (Infratec, Dresden, Germany), and a data processing and control system with digital signal processors for the spectrometer and the infrared camera. In the configuration used for this study, the spectrometer has an operating range between 680 and 3500 cm^{-1} (MCT detector) and a maximum spectral resolution of 0.2 cm^{-1} . The SIGIS system is schematically shown in Figure 1.

The operational principle of the SIGIS-HR for this application consists of placing the instrument at a safe distance from the aircraft's engine and acquiring infrared emission spectra around the exhaust plume. The analysis, which needs to be performed while the aircraft is stationary, can be done either in a test-bed or in real airport operating conditions. For completing an image of the gas plume with infrared spectral information, the scanning mirror is sequentially traversed over all positions (pixel-by-pixel) within the field view (FOV) specified by the user.

For fast visualization of the exhaust plume and brightness temperature of the background, a low-resolution mode (spectral resolution: 56 cm^{-1}) scan is performed. In this mode 17 interferograms per second are obtained and analyzed.

Each interferogram is recorded by the FTIR DSP system and the signal is Fourier-transformed. The resultant spectrum is analyzed by the DSP. In order to evaluate the brightness temperature of the exhaust gas, the integral of the spectrum in a spectral range that contains emission lines of the exhaust gas is calculated (for CO₂ a typical range is 2300 - 2400 cm⁻¹). To take into account the background temperature, the spectrum is analyzed in the range 800 - 1200 cm⁻¹.

The resultant spectrum is analyzed from which the brightness temperature of the exhaust gas is evaluated. For this and in order to avoid the influence of hot parts from the engine within the field-of-view, the integral of the radiance spectrum in a spectral range that contains emission lines of the exhaust gas is calculated. The false colour images of the calculated quantities are overlaid over the images of a video or infrared camera. Because the goal of this procedure is to locate the hottest part of the gas plume and background in the FOV, only a qualitative analysis is performed, i.e. no radiometric calibration is required.

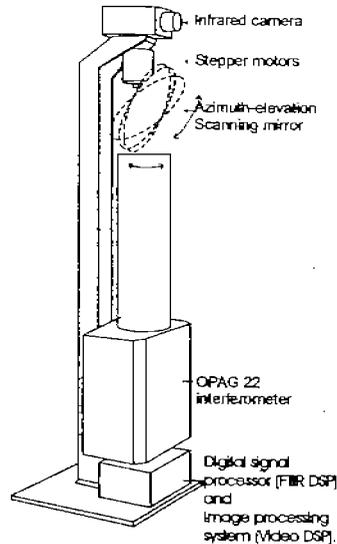


Figure 1. Schematic diagram of the Scanning Infrared Gas Imaging System (SIGIS-HR) for measuring temperature and gas distributions in turbine exhaust plumes.

Once the distribution of the brightness temperature is known, the next step is to record a high-resolution spectrum (0.2 cm⁻¹) in the position where the highest brightness temperature was detected. The spectra are averaged for at least 1 minute in order to achieve a satisfactory signal-to-noise ratio and then calibrated radiometrically against a black body at 200°C placed next to the instrument. The spectra are then further evaluated by a radiative transfer model (described below) in order to calculate the column densities of the gases.

In order to determine the ILS experimentally and to investigate the effect of the ILS on the retrieved column densities, a gas cell was mounted in front of the entrance window of the interferometer. The length of the stainless steel cell is 2 cm, the field of view is 5 cm, the material of the windows is BaF₂ and the windows are tilted by 2° to avoid reflection effects. The dimensions of the gas cell are given in Figure 2. All measurements were performed with a spectral resolution of 0.2 cm⁻¹ and no apodisation. The cell is filled with 2 % of CO in N₂ allowing an absorption of about 50 % of the incoming infrared radiation (0.3 absorbance units). The absorption cross section of the gas was calculated with the use of FASCODE (Smith et al., 1978)¹⁹ under conditions of the standard atmosphere (U.S. Standard Atmosphere, 1976)²⁰ based on the HITRAN database (Rothman et al., 2005)²¹. A black body of 200°C was used for the radiometric calibration. Moreover, the black body was used as radiation source behind the gas cell for the CO absorption measurement during

real ILS determination. An example of CO absorption spectrum at room temperature is given in Figure 3.

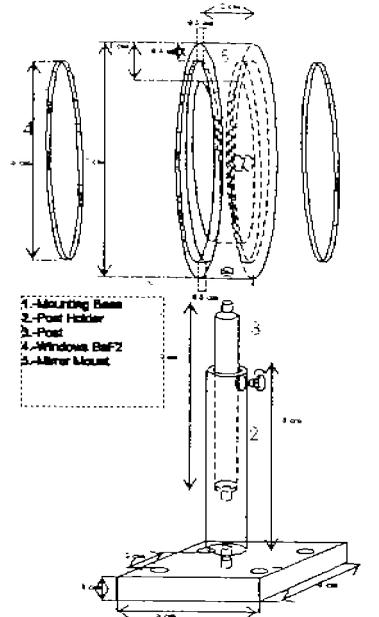


Figure 2: Cross-section of the CO gas cell at ambient air temperature.

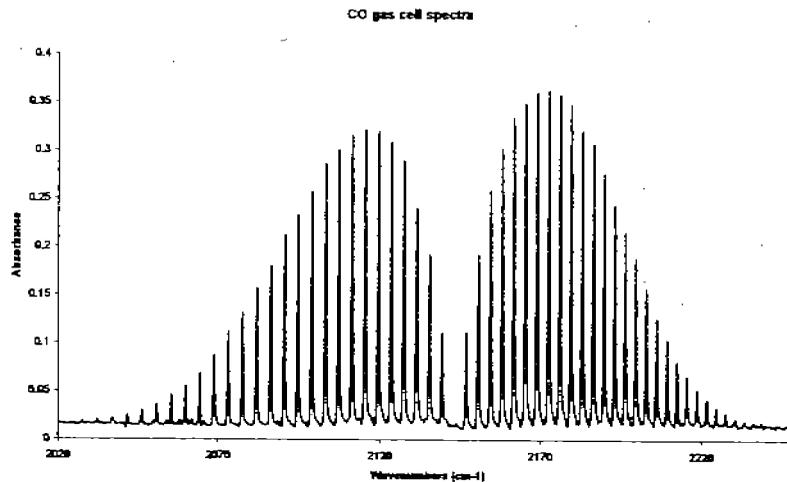


Figure 3: CO absorption spectra used for the ILS calculation.

Before and after the engine measurements the radiation of the black body is directed through the CO gas cell.

A software module was developed for completion of the Gedetekt software of SIGIS-HR which includes the model for the inherent apparatus function and the fitting algorithm on the basis of the measured spectra with the CO cell as described before is developed (Harig et al., 2005)¹⁶.

With the objective to observe the benefit of the inclusion of the new ILS into the software MAPS, two turbojet spectra were simulated using the original ILS (included into the first version of the software) and the new calculated ILS from the spectrometer SIGIS-HR plotted in the Figure 4. As result, the observed correlation factor between the simulated and measured spectra improved in both cases from 0.73 and 0.68 (using the ILS with the apodisation Norton-Beer-Strong) to 0.96 and 0.94 respectively (Figures 5 and 6).

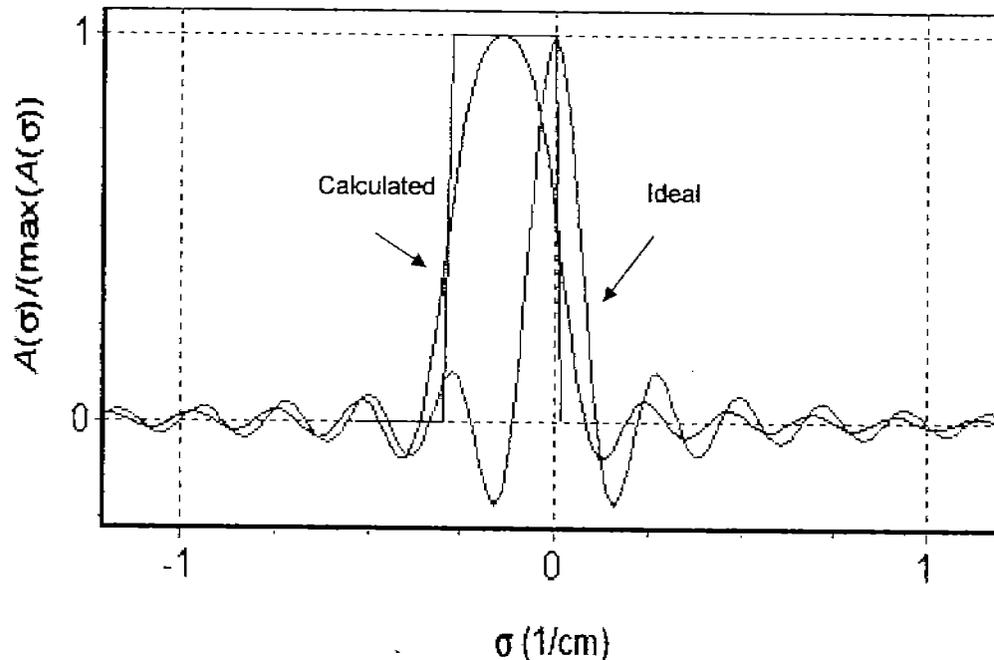


Figure 4: Ideal ILS (red) and measured ILS (blue) calculated by GeDetekt software using an absorption spectrum of CO at a concentration of 20000 $\mu\text{mol/mol}$.

3. MEASUREMENT RESULTS

The exhaust of a turbojet engine based on a Rolls-Royce Gnome 1200, originally operated in a Westland Wessex helicopter, was measured by the SIGIS-HR system. The power turbine and the duct which turns the exhaust 90 degrees in the helicopter installation had been removed from the engine and replaced by a straight jet pipe. Hence, the engine resembled a small turbojet engine with a higher exhaust temperature and velocity than would be encountered in the standard configuration of a Gnome.

To characterize the exhaust gas, a fast gas temperature scan was performed. As result, an important temperature difference between the upper and lower exhaust area was observed. This temperature difference, by itself represents an interesting result since engine designers can visualize in real time exhaust gas temperature asymmetries in the plume. Temperature asymmetries that may produce over heating effects on specific exhaust engine components can be investigated (see Figure 7).

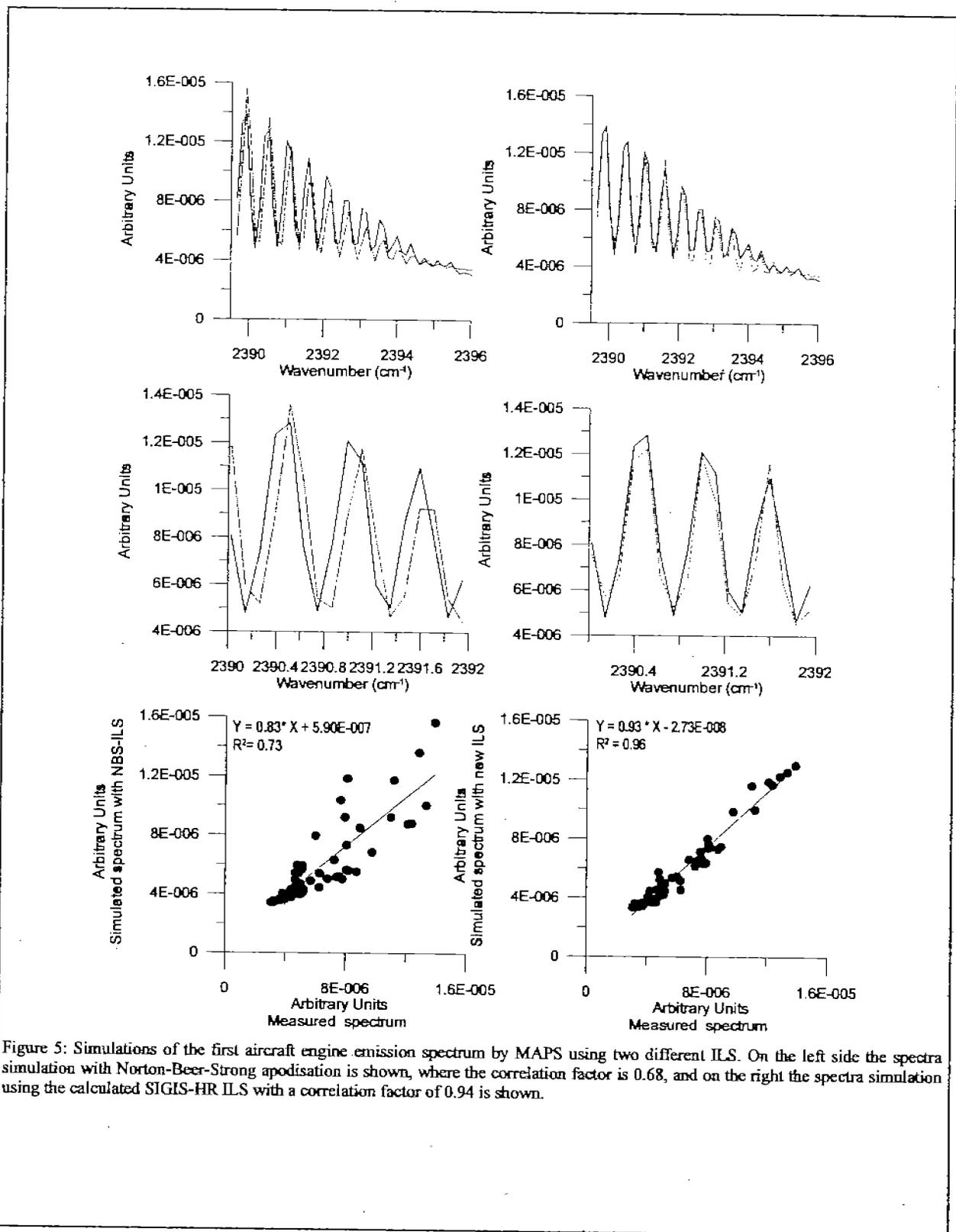


Figure 5: Simulations of the first aircraft engine emission spectrum by MAPS using two different ILS. On the left side the spectra simulation with Norton-Beer-Strong apodisation is shown, where the correlation factor is 0.68, and on the right the spectra simulation using the calculated SIGIS-HR ILS with a correlation factor of 0.94 is shown.

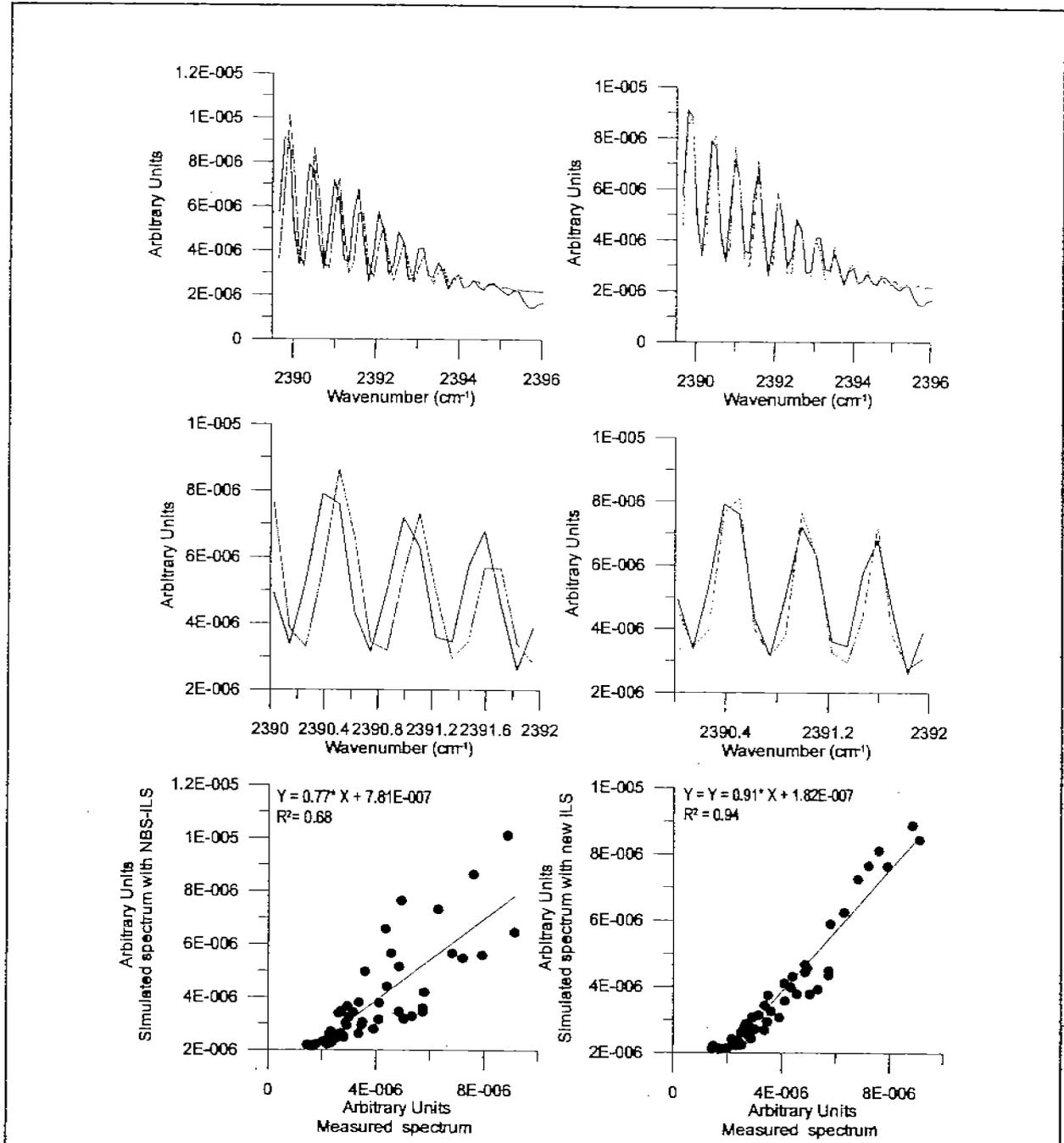
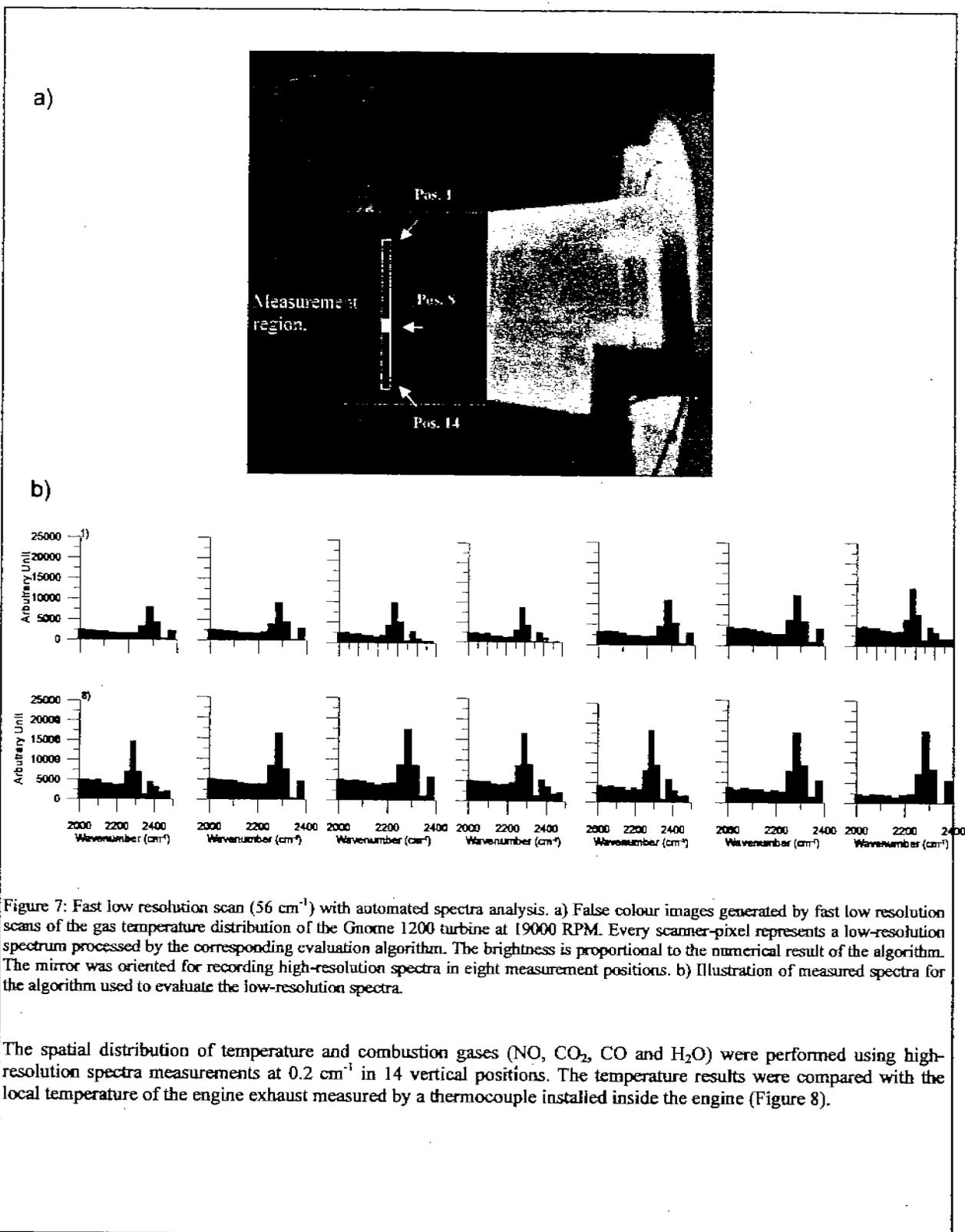


Figure 6: Simulations of the second aircraft engine emission spectrum by MAPS using two different ILS. On the left side the spectra simulation with Norton-Beer-Strong apodisation is shown, where the correlation factor is 0.73, and on the right the spectra simulation using the calculated SIGIS-HR ILS with a correlation factor of 0.96 is shown.



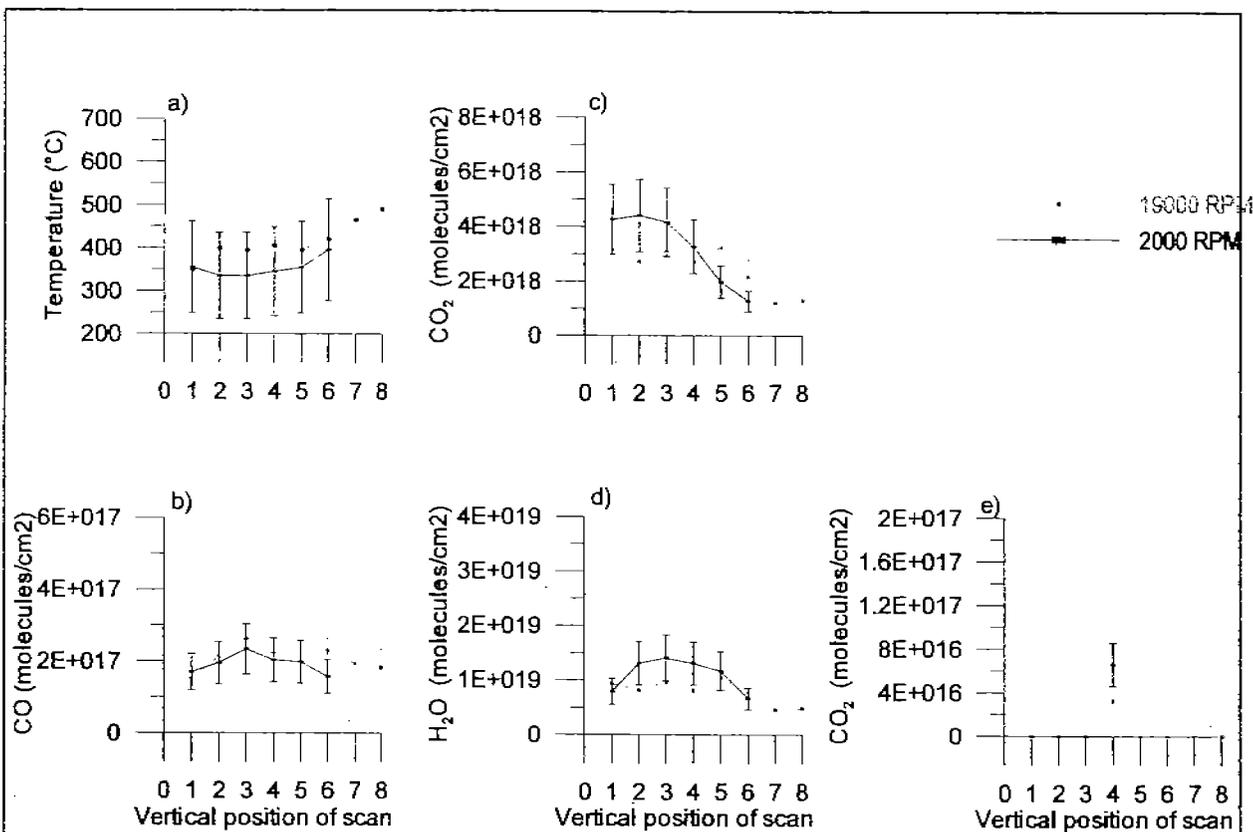


Figure 8: Vertical temperature (a) and CO, CO₂, NO and H₂O concentration profiles (b – d) of the turbine exhaust at an engine speed of 19000 and 20000 RPM. The error bars are $\pm 8^\circ\text{C}$ for the temperature graph and 4% for the concentration (e).

The average gas temperature calculated by MAPS at the power settings of 19000 and 20000 RPM were $436 \pm 130^\circ\text{C}$ and $353 \pm 106^\circ\text{C}$, respectively. The registered temperature by the thermocouple at the same engine power was 430°C and 365°C respectively, showing an important agreement between both independent measuring methods.

For CO, the average column density calculated at 19000 RPM was $2.08 \pm 0.62 \cdot 10^{17} \text{ cm}^{-2}$ and at 20000 RPM $1.93 \pm 0.57 \cdot 10^{17} \text{ cm}^{-2}$. The measurement uncertainty of the temperature and concentration calculations was considered as 30% as proposed originally by Heland, Schäfer (1997)². The origin of this important uncertainty value is due to the molecular data base uncertainty (HITEMP 15%) and the conversion of the molecular parameters at high temperature.

4. DISCUSSIONS

The calibration method presented in this work allows the determination of the ILS of mobile remote sensing FTIR spectrometry. The method is based on the measurement of the spectrum of a calibration gas in a small gas cell at ambient air temperature. Because of this simple setup, the method is applicable on-site. A well characterized ILS is a prerequisite for accurate results of retrieval algorithms. The presented model and the ILS determined by the method described allow the characterization of the ILS even if the instrument is not perfectly aligned or the ILS is degraded by aberrations. By including the real ILS of the SIGIS-HR system it was possible to improve substantially (from ~ 0.7 to 0.9) the correlation

between the measured and calculated spectra.

It was observed in the Gnome test bed measurements that the system allowed the detection of important differences in temperature and concentration in dependence from the engine operation and in the case of temperature measurements the calculated temperature results were consistent in all cases with the temperature measurement measured by thermocouple.

5. CONCLUSIONS

Scanning imaging FTIR emission spectrometry allows the characterisation of the spatial distribution of exhaust gas composition and temperature as well as quantifying the emission indices of aircraft engines. The system SIGIS-HR in combination with the new version of the software MAPS allows measurements in test beds. Among the advantages of performing measurements as described in comparison to the standard methods are:

- An excellent exhaust plume visualization that makes it possible for the operator to localize within a few seconds the exhaust plume.
- Easier high resolution spectra recorded by improvements in the localization and detection of infrared radiation.
- Possibilities to perform a thermo-scan that shows radiation temperature distribution anomalies of hot gas within the engine exhaust.
- No evidences of noise disturbance on the spectra during test bed and at airport measurements.

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