© EARSeL and Warsaw University, Warsaw 2005. *Proceedings of 4th EARSeL Workshop on Imaging Spectroscopy. New quality in environmental studies*.
Zagajewski B., Sobczak M., Wrzesień M., (eds)

ATMOSPHERIC MODELLING USING HIGH RESOLUTION RADIATIVE TRANSFER CODES AND IDENTIFICATION OF CO2 ABSORPTION BANDS TO ESTIMATE COALFIRE RELATED EMISSIONS

Prasun K Gangopadhyay, Freek van der Meer, Paul van Dijk

ESA Department
International Institute for Geo-Information Science and Earth Observation (ITC)
Hengelostraat, P.O. Box 6, 7500 AA Enschede, The Netherlands
Ph: +31 (0)53 4874248, Fax: +31 (0)53 4874336,
e-mail: prasun@itc.nl, vdmeer@itc.nl, vandijk@itc.nl

ABSTRACT

Recent studies of ice cores from Greenland and Antarctica have proven that both temperature and CO2 content of the earth's atmosphere followed a regular 100,000 year cycle of change and that they are closely correlated. Moreover, the observed increase of CO2 in the atmosphere exceeds the predicted values extrapolated from historical data. Other than industrialization and rapid urbanization, geo-natural hazards such as spontaneous combustion of coal contribute a considerable amount of CO2 to the atmosphere. To establish a functional environmental model, it is important to quantify the amount of Green House Gas (GHG) emissions on a local scale. Radiative transfer codes, such as FASCOD (Fast Atmospheric Signature Code) with HITRAN2K (High Resolution Transmission) spectral database can simulate atmospheric transmission and path radiance with customized gas composition (CO2, water vapour, CO etc.) and concentration to understand the phenomena in a specific wavelength region. In the present study a number of atmospheric models were simulated with different CO2 concentrations (ppmv) with combination of water vapour and other atmospheric gases such as CO, CH4, N2O, SO2 etc., to find out the interference patterns of these gases over CO2 absorption bands. The transmission features of these gas combinations were analysed by partial least square regression models. These models show that the most suitable CO2 absorption bands are located around 2μm such as 2.0086, 2.0095, 2.0101μm. The spectral information derived from different concentrations of CO2 can be fitted in multivariate models to predict the CO2 concentration from spectral information in a controlled environment.

Keywords: radiative transfer code, FASCOD, transmittance, CO2 absorption band, environmental modelling

INTRODUCTION

Over the past two centuries, anthropogenic emissions of greenhouse gases (GHG) have increased to an alarming situation. This steadily increment of GHGs in atmosphere act as a blanket that retains solar radiation in the atmosphere and led to global warming. Among the all GHG, CO2 has a significant status in this phenomenon. Since pre-industrial era the concentration of CO2 has increased from 280 ppm to 350 ppm. This linear increment of concentration of CO2 is not only influenced by human activity such as rapid industrialization, deforestation but also some geo-natural events e.g. coalfire.

In most coal-producing countries subsurface and surface coal fires are a serious problem, which is evident in China, India, Indonesia etc. Considerable economic and environmental problems are directly related to coalfires. Apart from consuming a valuable resource, it emits an enormous amount of sulfur dioxide, nitrogen oxides, carbon monoxide and carbon dioxide depending on the size and spread of the fire. It has been studied that the CO2 emissions from only Chinese coalfires contributes about 0.3% of total CO2 emitted from fossil fuels (Voigt *et al*., 2004).

Borehole temperature measurements were the main tool to detect subsurface coalfires until the 1960s. During the early sixties when airborne thermal scanner data and later satellite borne thermal scanner data started to become available, remote sensing based coalfire detection and monitoring became possible. Such studies in the United States, Australia, India and China were carried out by concentrating on coalfire detection, monitoring, depth estimation and thermal modelling using spaceborne and/or airborne thermal data.

To simulate the customised atmosphere, PcLnWin or commercial version of FASCOD3P, is a useful tool. PcLnWin performs calculations from the ultraviolet through the visible, infrared & microwave spectrum (0-50000cm-1). This radiative transfer model accommodates atmospheric profiles, numerous aerosol models, water and ice cloud models. Spherical refractive geometry calculations are performed for any arbitrary line of sight chosen. PcLnWin performs line by line calculations using spectroscopic parameters obtained from the HITRAN.

High spectral resolution imaging spectrometers provide relatively narrow-band measurements in a spectral region that contains absorption features caused by atmospheric gases. Several imaging spectrometers are in use in different characteristics (Goetz, 1991). Hyperspectral instruments such as AVIRIS can be useful for observing gas concentrations in specific wavelength (Gao and Goetz, 1990; Schlapfer *et al* 1998). Most of these sensors typically have a band width of ~10nm covering the whole visible and some part of the short-wave infrared region.

The preset study aims to establish the relation between transmission and concentration of CO2 (ppmv) in a controlled atmosphere.

METHOD AND DISCUSSION

Coalfire detection and monitoring

A surface having a temperature more than absolute temperature emits energy, depending on the properties of the surface and is function of the wavelength. Emissivity is an inherent property of surface and is independent of irradiance. Planck's law describes the relation between the temperature and radiance of a perfect emitter (black body). The thermal anomalies above the underground coal fires can be detected by different remote sensing sensor such as Landsat TM/ETM, ASTER, MODIS and some dedicated missions such as BIRD and FOCUS. The TES algorithm, developed by the ASTER team, can extract temperature and emissivity (Gillespie *et al.*, 1999) using multispectral thermal data. There are many methods are developed by researcher such as RCM (reference channel method), NEM (normalized Emissivity method) etc.

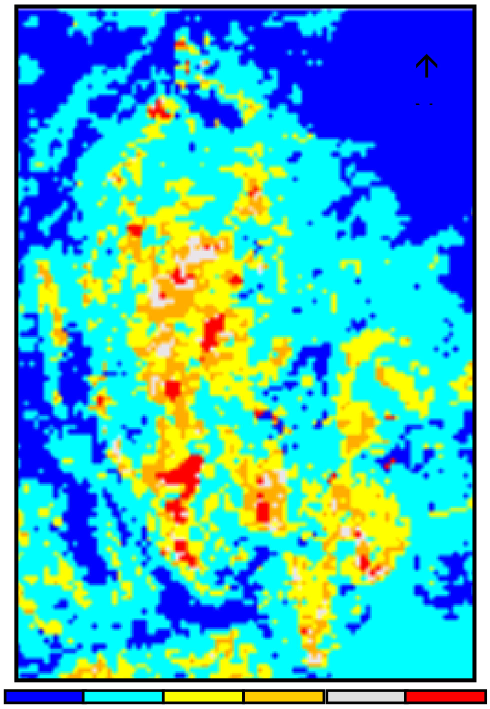

Fig. 1: *Isothermal zonation of a test area, red patches are identified as coalfires*

These methods along with ASTER thermal data were used in a test area in northern China and found very useful to extract the thermal anomalies due to coalfires with the inputs from local geological map (Fig. 1).

Radiative transfer in atmosphere

The quantitative study of the transfer of radiant energy through a medium which can scatter, absorb and emit radiation is referred as radiative transfer theory. In the field of remote sensing and atmospheric science it has significant applications. Till date many methods concerning radiative transfer in atmosphere are proposed, such as Eddington approximation (Shettle and Weinman, 1970), the F_N method (Garcia and Siewert, 1989), the discrete ordinates method (DOM) (Liou, 1973; Stammes and Dale, 1981; Stammes and Conklin, 1984; Stammes et al, 1988) Monte Carlo method (Collins *et al*, 1972), the spherical harmonics method (Dave, 1975; Benassi *et al*, 1984). PcLnWin or commercial package of FASCOD3P calculates spectral transmittance, radiance, or optical depth for a given path by using line-by-line calculation for very high spectral resolution. FASCOD3P uses line-by-line calculation algorithm with continuum models, a spherical refractive geometry package and standard atmospheric and aerosol profiles to provider a real world atmospheric models. Spectral lines (emission or absorption) occurs at very specific monochromatic frequencies, but in reality these single frequency emissions are broadened by both collisions with other molecules and by Doppler's shifts caused by the velocity of the radiating molecule. In the present study FASCOD3P was used with combination of HITRAN2K spectral database to simulate atmospheric models.

The HITRAN2K database includes 32 molecular species along with values of cross-sections of heavy molecules such as CFCs (Vanarasi and Nemtchinov, 1994). The spectral absorption, transmission and emission of radiation in the atmosphere are influenced by the shape, location and intensity of the absorption line. The HITRAN database provides line position (cm-1), the intensity of the transition (cm-1 molec-1 cm2), air-broadened half width (cm-1 atm-1) and the energy of the lower state of the transition (cm-1).

Coalfire and related gaseous emissions

Most of the coalfire related studies are focussed on detection and monitoring using remote sensing as a prime tool. But the emission from these coalfires has a deep impact in local and global environment. The gaseous emissions from coalfire, not only pollute the local atmosphere, but also add substantial amounts of the greenhouse gases (CO_2, CH_4) along with the SO_x, NO_x and CO. Among the all emitted gases CO2 has worst impact on environment because of its higher quantity. A base line inventory of the CO_2 emissions from the coal fires could reflect the present and the future projected scenario for a better management of coalfire.

Detecting CO2 absorption bands to estimate emissions from coalfires

To identify the discrete CO2 absorption lines, two types of atmosphere were simulated using FASCOD considering the atmospheric conditions expected in the proposed study area. The first simulated atmosphere consists of only CO2 i.e. without water vapour, other atmospheric gases and aerosol and the other one is consist of all atmospheric constituents except CO2. Later these two data sets were resampled in 1nm resolution to understand the phenomenon in the range of 700-2500nm that covers most of the hyperspectral remote sensing sensors.

From Fig. 2 it is evident that energy is being influenced by all atmospheric constituents though out the spectrum other than 2000nm. Around 2000nm the energy is absorbed by a strong CO2 absorption band only. The close-up of that part of spectrum (1858-2048nm) has shown in figure 2 for a better understanding. Here red and blue line represents CO2 (360ppmv) and all other atmospheric constituents respectively.

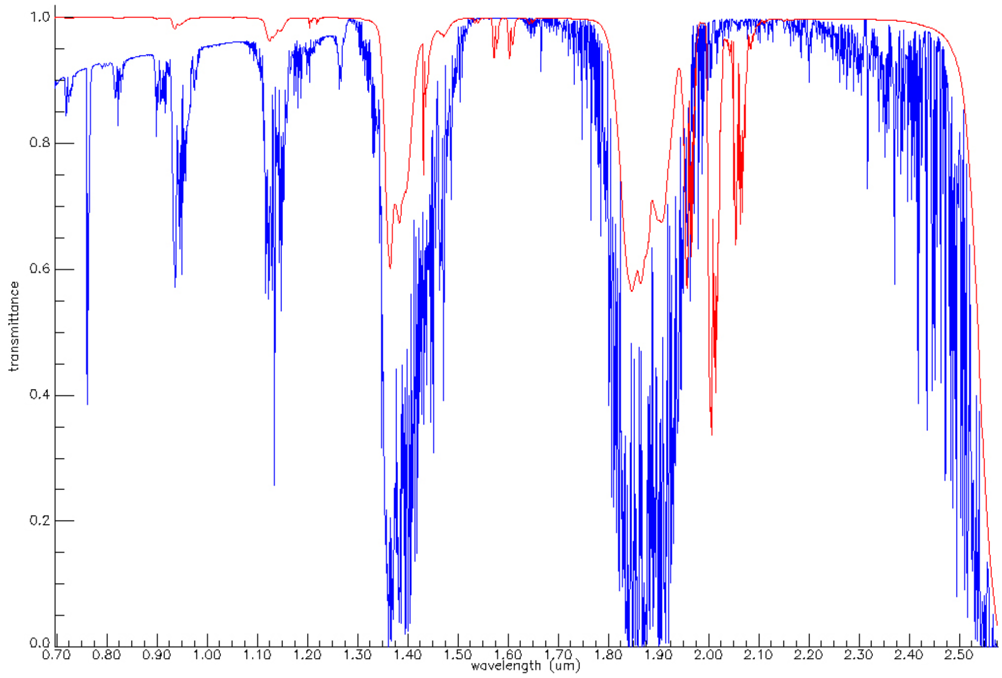

Fig. 2*: Absorption of CO2 (red and other atmospheric gases (blue) in the wavelength region of 0.7-2.5μm*

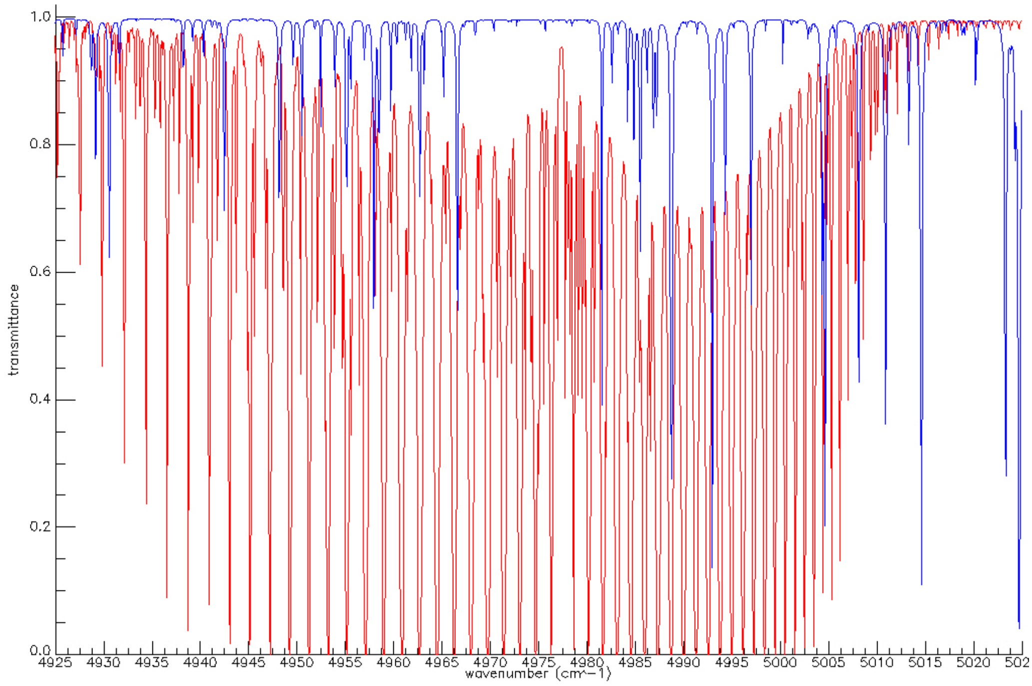

***Fig. 3**: CO2 (red) and other atmospheric gases (blue) absorption lines in the wavenumber region of 4925-5025cm-1*

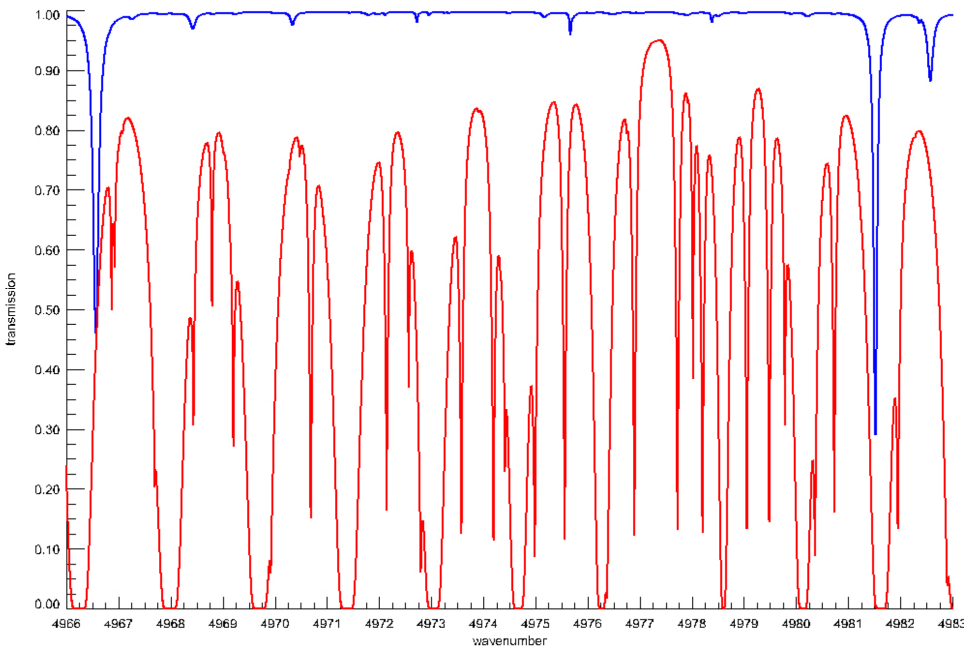

***Fig. 4**: Distinct CO2 (red) absorption lines in the wave number region of 4968-4980cm-1*

As seen in the Fig. 4 the whole range of spectrum, apparently has very less influence of atmospheric gases other than very frequent existence of CO2 lines. In the middle of this region, i.e. 2.0083nm (4980cm-1) to 2.013nm (4968cm-1), the energy is only influenced by CO2.

The detailed view of figure 3 shows that very strong CO2 absorption lines are present in 2008, 2008.6, 2009.5, 2010.2, 2010.1, 2011.5, 2012.2 and 2012.9nm (4980.14, 4978.62, 4976.24, 4974.67, 4973.05, 4971.38, 4969.71 and 4968cm-1) which are not influenced by other atmospheric gases significantly.

To estimate the significance of these absorption bands, partial least square method (PLS) was used with different concentrations of CO2 (330ppm to 570ppm) in the same wavelength region.

Among the significant bands three absorption bands were chosen which are not influenced by any other atmospheric constituents such as water vapour. These three bands are situated in 1.998, 2.001 and 2.01 μm (Fig. 5).

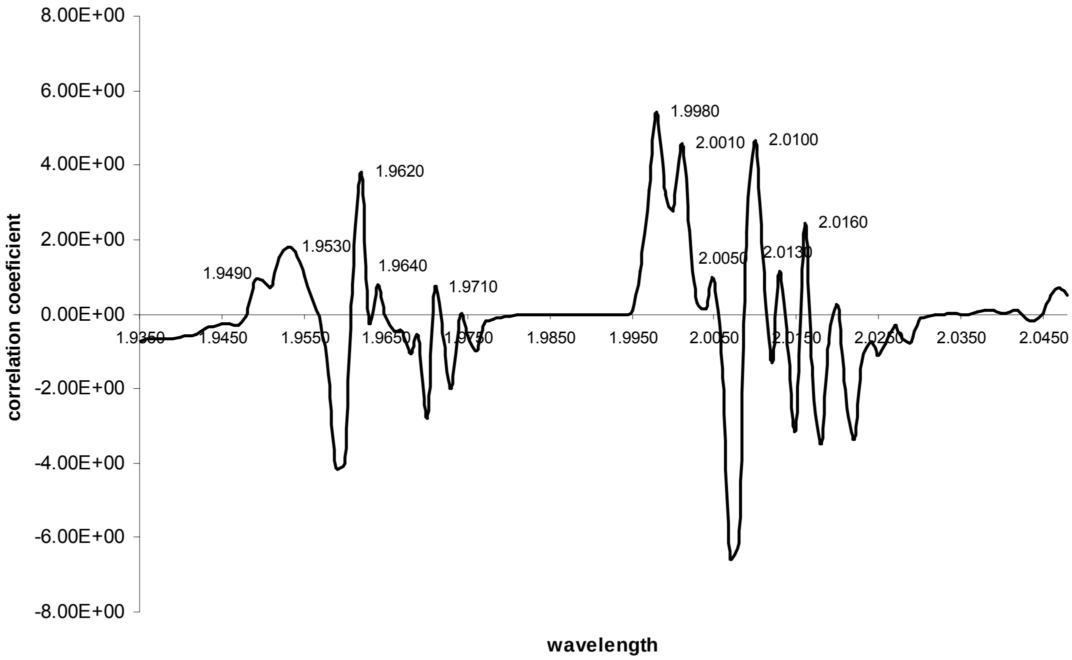

***Fig. 5**: Distribution of significant CO2 absorption bands*

Later, these three particular absorption bands were tested with different concentrations of CO2 to find out their sensitivity with changing gas concentration. As seen on the figures (Fig. 6a, 6b and 6c) there is a good relation between CO2 concentration and transmission.

Also with different concentrations (ppmv) of CO2 were used to simulate atmospheric models to understand how much it can influence the energy in that particular region. As seen in the following figure (Fig. 7), the transmittance has decreased with the increment of CO2 concentration and in the case of 48000 ppmv (as in analyzed gas sample, collected from a vent in a coalfire in northern China), the transmittance value decreased drastically.

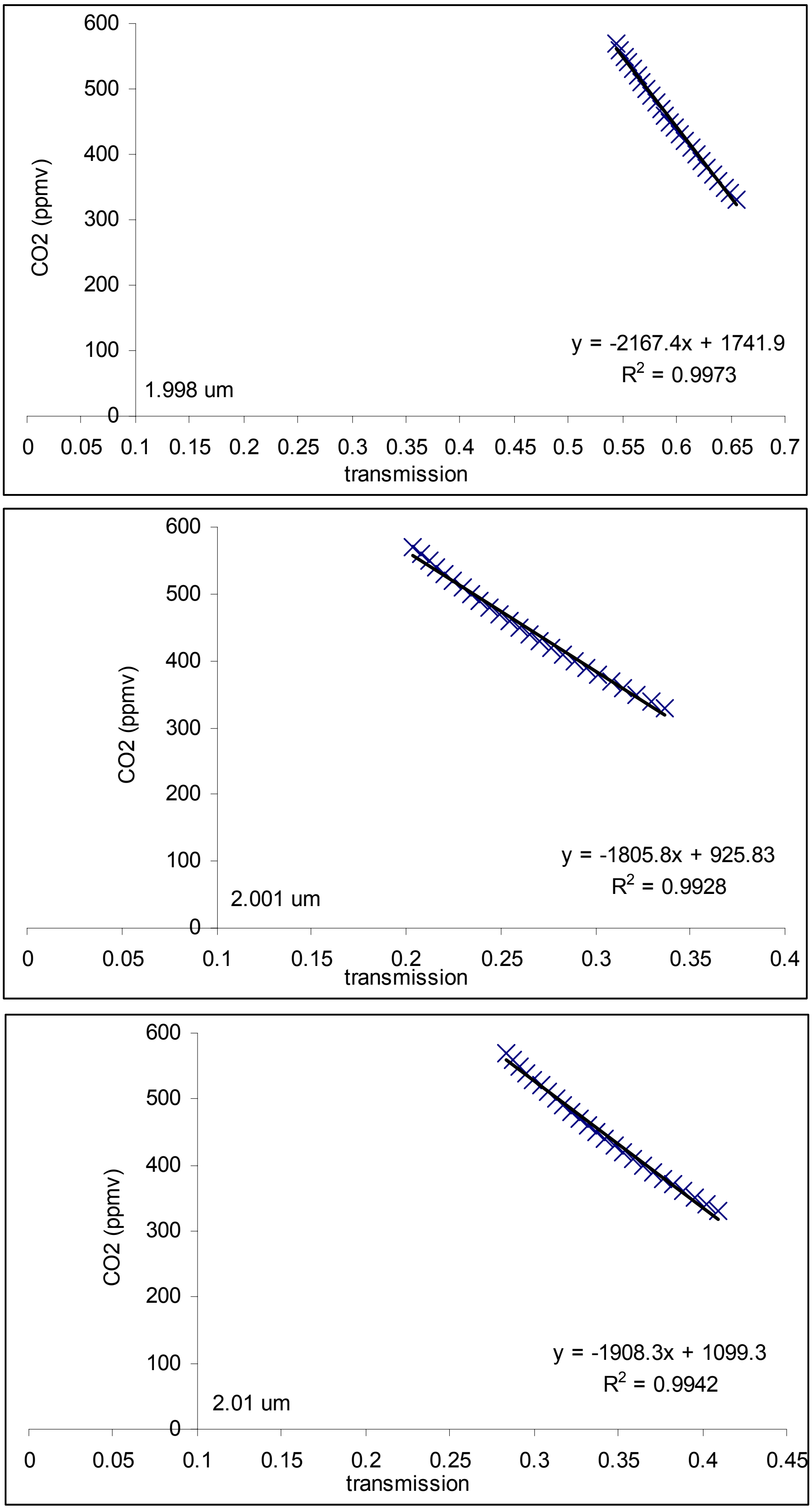

Fig. 6a, 6b, 6c: The relation between CO2 concentration and transmission in three selected wavelength in controlled atmosphere

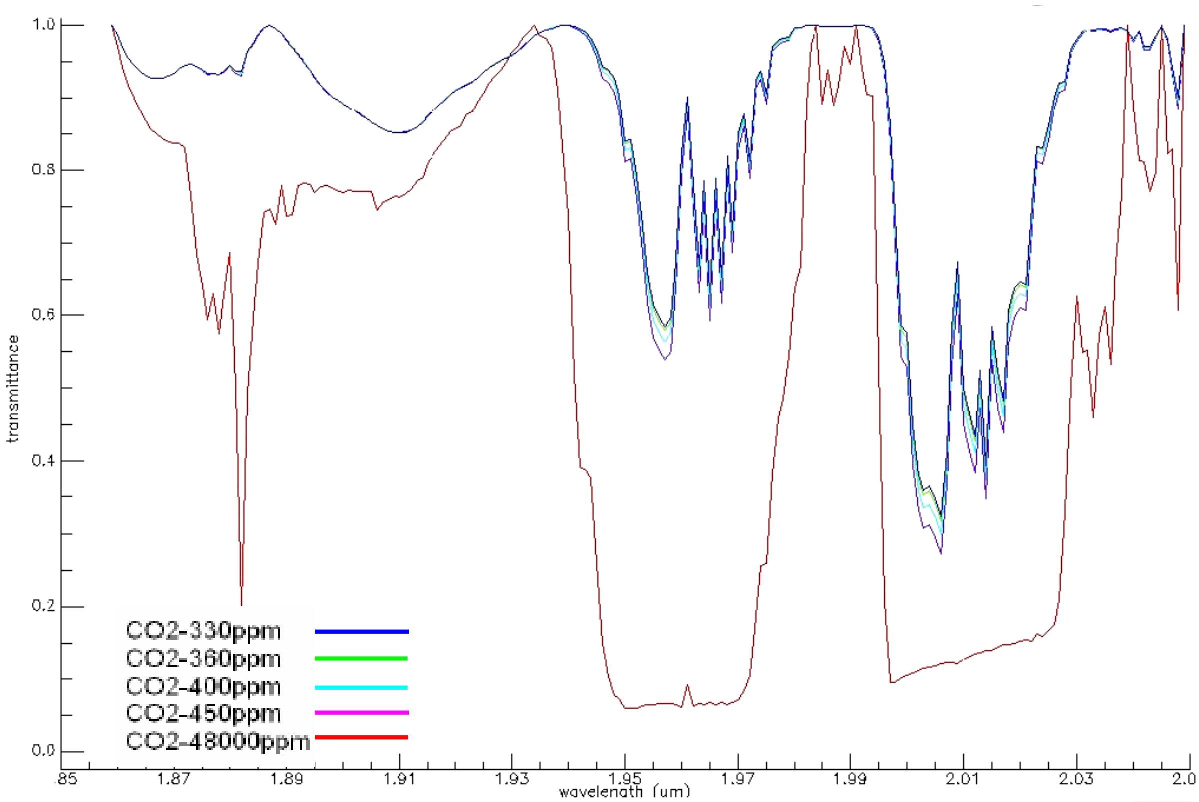

Fig. 7: Model runs of radiative transfer through atmosphere profiles with different CO2 concentrations. Note the increase of CO2 related absorption features with increasing concentration.

CONCLUSION

Coalfire is a wide spread problem in most coal producing countries. To detect and monitor coalfire, remote sensing is playing a significant role to prevent huge economic loss and environmental disaster. The green house gases emitted from coalfires is needed to be considered more seriously as coalfire related green house gases have a significant adverse contribution to global climate. As seen in the present study the relation between transmission and concentration of CO2 can be extended to radiance at sensor and concentration of CO2 by inversion method. Though the most hyperspectral instruments operate in visible and shortwave infrared range where the absorption bands of CO2 is very narrow, still there is an option to scale down the parameters retrieved from models (laboratory based) and fit in the available remote sensing bands.

Reference

Benassi, M.,Garcia, R.D.M., Karp, A. H. and Siewert, C. E., 1984. A high-order spherical harmonics solution to the standard problem in radiative transfer. *Astrophys. J.*, 280, 853–864

Collins, D. G., W. G. Blattner, M. B. Wells, and H. G. Horak., 1972. Backward Monte Carlo Calculations of the Polarization Characteristics of the Radiation Emerging from Spherical-Shell Atmospheres, *Appl. Opt.*, 11 (11), 2684-2696.

Gao, B.C. and Goetz A.F.H., 1990. Column Atmospheric Water Vapor and Vegetation Liquid Water Retrievals From Airborne Imaging Spectrometer Data, *J. Geophys. Res.*, 95 (D4, pp. 3549-3564.

Garcia R.D.M. and Siewert, C.E., 1989. On discrete spectrum calculations in radiative transfer, *J. Quant. Spectrosc. Radiat. Trans.*, 42, 385-394.

Gillespie, A. R., Rokugawa, S., Hook, S.J., Matsunaga, T. And Kahle, A.B., 1999. Temperature/Emissivity Separation Algorithm Theoretical Basis Document, Version 2.4, Prepared under NASA Contract NAS5-31372, 8-5.

Liou, K.N., 1973. A numerical experiment on Chandrasekhar's discrete-ordinate method for radiative transfer: Applications to cloud and hazy atmospheres. *J. Atmos. Sc.*, 30, 1303-1326

Schläpfer, D., Keller, J., and Itten, K.I., 1997. Retrival of horizontal and the vertical water vapor distribution from AVIRIS data. In *7th Int. Symp.Phys. Meas. Sig. Rem. Sens.*, ISPRS, Courchevel (F), II,591-598.

Shettle, E. P. and J. A. Weinman, 1970. The transfer of solar irradiance through inhomogeneous turbid atmospheres evaluated by Eddington's approximation. *J. Atmos. Sc.,* 27, 1048-1055.

Stamnes, K. and Dale, H., 1981. A New Look at the Discrete Ordinate Method for Radiative Transfer Calculations in Anisotropically Scattering Atmospheres. II: Intensity Computations, *J. Atmos. Sci.*, 38, 2696-2706

Stamnes, K. and P. Conklin, 1984. A New Multi-Layer Discrete Ordinate Approach to Radiative Transfer in Vertically Inhomogeneous Atmospheres, *J. Quant. Spectrosc. Radiat. Trans.,* 31, 273-282.

Stamnes, K., Tsay, S. E., Wiscombe, W. and Jayaweera, K., 1988. A Numerically Stable Algorithm for Discrete-Ordinate-Method Radiative Transfer in Multiple Scattering and Emitting Layered Media, *Appl. Opt.*

Varanasi, P. and Nemtchinov, V., 1994. Thermal infrared absorption coefficients of CFC-12 at atmospheric conditions. *J. Quan. Spectrosc.Radiat. Trans.*, 51, 679-687

Voigt, S., A. Tetzlaff, J. Zhang, C. Künzer, B. Zhukov, G. Strunz, D. Oertel, A. Roth, van Dijk P. and Mehl H., 2004. Integrating satellite remote sensing techniques for detection and analysis of uncontrolled coal seam fires in North China. *Int. J. Coal Geo.*, 59, 121-136.

Yamamoto, G., 1962. Direct Absorption of Solar Radiation by Atmospheric Water Vapor, Carbon Dioxide and Molecular Oxygen, *J. Atmos. Sc.*, 19, 182-188.