

FT-IR as process analytical technique for Post Combustion Capture

Leon F. G. Geers^a, Annemieke van de Runstraat^a, Ralph Joh^b, Rüdiger Schneider^b, Bertus Bergsma^a and Earl L. V. Goetheer^a

^aTNO, Leeghwaterstraat 46, 2628 CA Delft, The Netherlands

^bSiemens, Industriepark Hoechst, G811, 65926 Frankfurt-am-Main,
earl.goetheer@tno.nl

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Introduction

One of the possible ways to reduce our carbon footprint is using post-combustion capture (PCC) processes to remove CO₂ from flue gases. Due to the highly dynamic character of such processes, real-time performance monitoring is a very complex task. This paper presents a method for monitoring the concentrations of CO₂, SO_x, and a CO₂ capturing agent (b -alanine) during a process in a PCC pilot plant. A partial least squares (PLS) model was built to estimate these concentrations from Fourier transform infrared (FTIR) spectra of the capturing solvent during processing in a model PCC plant. The model predicts the species concentrations to within 0.05 mol/l, provided the concentrations stayed within the calibration window of the model. Eventually, the model was used to monitor an emulated PCC process on-line during 24 hours of processing. This showed that events such as saturation of the capturing agent with CO₂, water replenishment, and switching to safety protocols can be followed accurately.

Tool development

FT-IR spectroscopy is a method to identify different chemical species based on the absorption of light of specific wavelengths. Different chemical bonds absorb energy at specific wave lengths. The height of the absorption peaks in the spectrum is related to the molecular concentration of species. The challenge for using FT-IR spectroscopy as a monitoring tool for PCC is that the different species present in the solution interact with each other and with water. Moreover, the peaks of the different species overlap, so there is no one-to-one relation between the height of specific peaks and species concentrations.

The field of chemometrics offers a more sophisticated data analysis method that enables the independent determination of species concentrations from spectra of mixtures. Partial least squares regression (PLSR) was specifically developed to handle modelling problems with more variables (i.e. data points in a spectrum) than observations (i.e. species concentrations), since they cannot be handled by ordinary linear regression. In PLSR, a calibration model is constructed on the basis of a set of mixtures with known concentrations and spectra. This model describes the individual contribution of each species to the spectra of the mixtures. Hence, it can be used to dissect spectra of unknown mixtures of the same species to reveal their concentrations.

Calibration and validation of the model

In order to calibrate and validate the model for the relevant PCC species, 52 stock solutions were made. These solutions each contained different concentrations of the capture solvent, CO₂, and SO₂, within the ranges expected during process operation. Of the 52 solutions, 37 were used to construct the PLSR model and the remaining 15 were used to validate it. The model was able to predict the concentrations of the three species within 3% of the measured values..

Microplant tests

The in-line applicability of the method was assessed in a microplant (Figure 1a). This is a lab-scale pilot plant mimicking the PCC plant, but without the SO₂ scrubber. It is fed with artificial flue gas (air with CO₂) and it is operated continuously and automatically. A flow-cell is connected to either the rich or the lean stream. The FT-IR spectrometer then continuously takes spectra from the fluid passing the flow-cell, and the PLSR model converts the spectra into concentration values. In Figure 1b an example is given.



Figure 1a: microplant

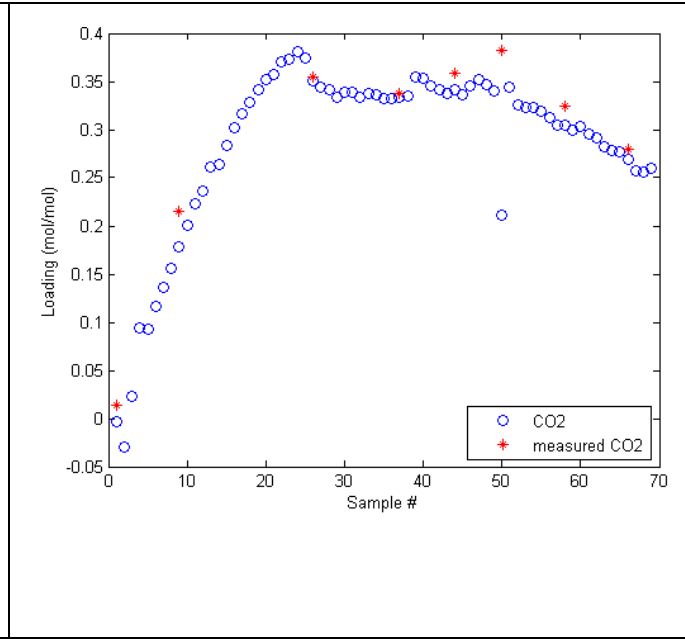


Figure 1b: an example: continuous measurement of rich liquid during CO₂ absorption

It can be concluded that the combination of an FTIR spectrometer and a PLS model can be used to extract process information in real-time. This is a valuable tool for the continuous measurement of the different components present in a post-combustion capture process. Based on this tool control systems can be designed.