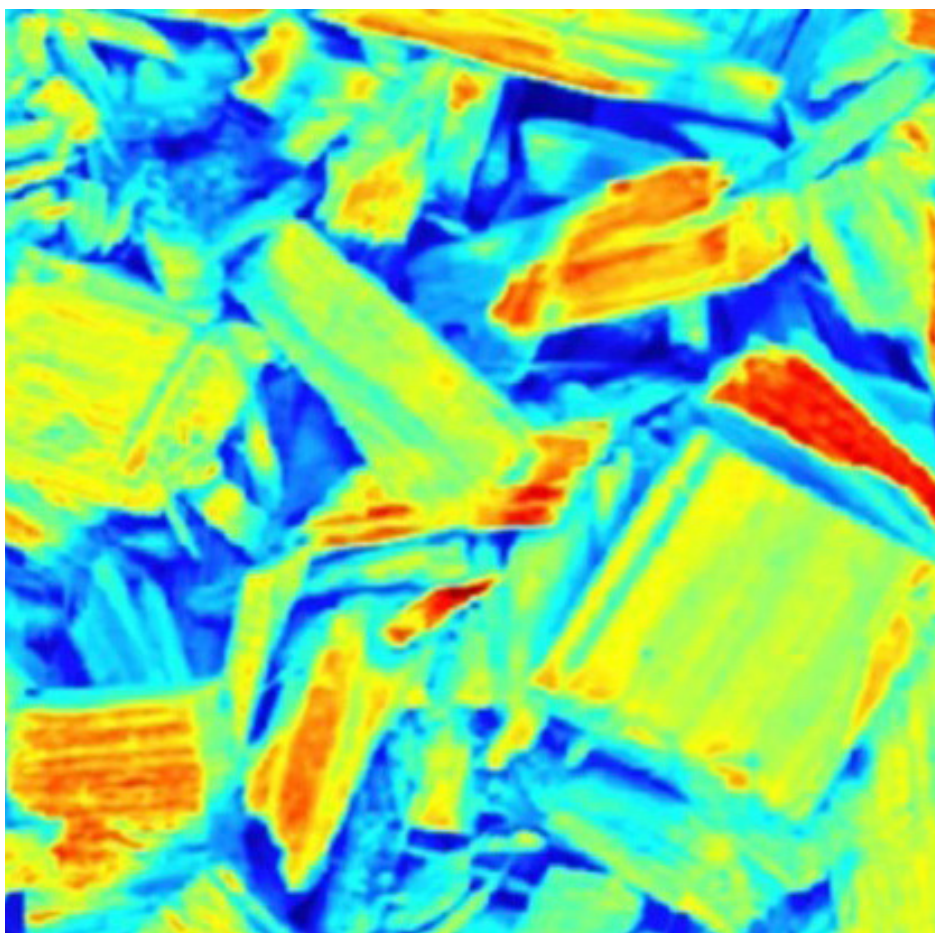


ON-LINE POWERPLANT CONTROL USING NEAR-INFRARED SPECTROSCOPY

REPORT 2021:746



On-line Powerplant Control using Near-InfraRed Spectroscopy

OPTiC-NIRS

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Förord

Denna rapport är slutrapportering av projekt 44912 OPTiC-NIRS – On-line styrning av kraftverk med närainfraröd spektroskopi (Energimyndighetens projektnummer P 44912).

Projektet har finansierats av Energimyndigheten och av de organisationer som utgjort industriparterna i SEBRA (samverkansprogrammet för bränslebaserad el- och värmeproduktion). Dessutom har Eskilstuna Strängnäs Energi och Miljö, Mälarenergi, First Control, Bestwood och ENA Energi bidragit med naturinsatser.

SEBRA-programmets övergripande mål har varit att bidra till långsiktig utveckling av effektiva miljövänliga energisystemlösningar. Syftet är att medverka till framtagning av flexibla bränslebaserade anläggningar som kan anpassas till framtida behov och krav. Programmet fyra teknikområden: anläggnings- och förbränningsteknik, processtyrning, material- och kemiteknik samt systemteknik. Detta projekt hör till teknikområde Anläggnings- och förbränningsteknik.

Målet med projektet har varit att utvärdera potentialen att använda NIR-mätningar som soft sensors för online-karaktärisering av biomassa och avfallsmaterialegenskaper för diagnostik och optimal kontroll av kraftvärmeverk.

Projektet har genomförts vid Framtidens energi (Future Energy Center) vid Mälardalens Högskola i Västerås. Konstantinos Kyprianidis har varit huvudprojektledare med ett projektteam bestående av Mikael Karlsson, Robert Tryzell, Ioanna Aslanidou, Erik Dalhquist, Jerol Soibam, Jan Skvaril, Martin Şevçik, Nathan Zimmerman, Milan Zlatkovikj, Philip Hedlund och Elena Tomas Aparicio.

Från Energiforsks sida har projektets följts och utvärderats av en referensgrupp bestående av Tania Irebo (Swerim), Fredrik Axby (Sweco), Hans Larsson (Stockholm Exergi) och Henrik Harnevie (Vattenfall).

Stockholm mars 2021

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Områdesansvarig
Termisk energiomvandling, Energiforsk AB

Authors foreword

The OptiC-NIRS project, On-line Powerplant Control using Near-InfraRed Spectroscopy, has been led by Prof Konstantinos Kyprianidis. The work has been carried out at the Future Energy Center at Mälardalen University in Västerås, Sweden.

The integrated MDH team included: Mr Mikael Karlsson, Dr Robert Tryzell, Dr Ioanna Aslanidou, Prof Erik Dalhquist, Mr Jerol Soibam, Dr Jan Skvaril, Mr Martin Sevçik, Mr Nathan Zimmerman, Mr Milan Zlatkovikj, Mr Philip Hedlund and Ms Elena Tomas Aparicio.

The project has been funded by Energiforsk and Energimyndigheten. Eskilstuna Strängnäs Energi och Miljö, Mälarenergi, First Control, Bestwood, and ENA Energi are acknowledged for their in-kind co-financing and contributions that have enabled this work.

Finally, we are particularly thankful to all the members of the OptiC-NIRS project reference group (Fredrik Axby, Sweco; Tania Irebo, Swerim; Hans Larsson, Stockholm Exergi; Henrik Harnevie, Vattenfall) for the inputs provided during the course of the project and in the preparation of this technical report.

These are the results and conclusions of a project, which is part of a research programme run by Energiforsk. The author/authors are responsible for the content.

Sammanfattning

Karakterisering av biobränsle har stor betydelse för energibranschen. I dag sker det framförallt i form av ankomstkontroll av bränsleleveranser där fokus ligger på fukthalt och askhalt. OptiC-NIRS projektet har studerat on-linekarakterisering i syfte att kunna styra och kontrollera förbränningsprocesserna inom kraft- och värmebranschen. Det är ett antal olika egenskaper i bränslet som är av intresse för processen. Fukthalt i biobränslet har en direkt påverkan på processen på ett antal olika sätt i realtid och att erhålla information on-line om fukthalten skapar direkt möjligheter att direkt styra processen mot en bättre bränsleekonomi. Andra egenskaper som också är av vikt är värmevärde, askhalt, innehåll av glas och innehåll av fossilt material såsom plaster.

Det övergripande målet med projektet var att utvärdera potentialen att använda NIR mätningar som mjuka sensorer för karaktärisering on-line av egenskaper hos biomassa och RDF. En kombination av laboratorieexperiment och demonstration i full skala utfördes framgångsrikt.

Genom att erhålla information om dessa egenskaper skapas inte bara möjligheter till en effektivare förbränning utan också möjligheter att minska emissioner av oönskade ämnen. Genom att i realtid få information om fukthalten på bränslet kan en stabilare förbränningstemperatur erhållas och därmed en reduktion av bildandet av NO_x. Vid sopförbränning är andelen glas i bränslet viktig för att undvika sintring av bädden, andelen plast (fossilt) är viktig av regulatoriska skäl och speciellt andelen klorinnehållande plast som kan leda till bildandet av dioxiner.

För att möjliggöra denna karakterisering har olika spektroskopiska sensorer studerats, framför allt NIR (Nära Infraröd) spektroskopiska metoder. De olika mjuka sensorer (soft-sensors) som har studerats inom projektet har spänt från traditionell FT-NIR och DA-NIR till HSI (Hyperspectral NIR Imaging), även Raman NIR spektroskopi med två olika lasersystem har undersökts men visade sig ej vara lämpade för denna applikation. De olika teknikerna har olika för- och nackdelar vid bestämning av de olika egenskaperna i realtid on-line.

OptiC-NIRS projektet har utförts i två olika faser, en laboratoriefas där de olika teknikerna studerades med avseende på de egenskaper som skulle bestämmas vid SPECTRA-lab på Future Energy Center på Mälardalens Högskola i Västerås och en anläggningsfas där de mest lovande teknikerna implementerats och demonstrerats on-line vid Mälarenergi i Västerås och vid Eskilstuna Strängnäs Energi och Miljö i Eskilstuna.

Gemensamt för de NIR tekniker som använts är att de kan användas on-line utan uttag och uppärbetning av prov vilket gör sensorerna mycket lämpade för realtidsmätning on-line. Däremot så kräver metoderna att de tränas, kalibreras, för de egenskaper som skall bestämmas. Denna kalibrering har skett dels på SPECTRA-lab och dels på de anläggningar där sensorerna testats. Råsignalen, spektra, från de olika instrumenten kan förenklat liknas vid kemiska fingeravtryck

från biobränslet. För att skapa kalibreringsmodeller mäts det på ett referensprov som sedan får analyseras för de önskade egenskaperna därefter byggs en matematisk modell som korrelerar den kemiska informationen i spektra med de värden som referensmetoden ger. Då biobränsle är ett mycket heterogent material, stora variationer med avseende på olika parametrar, krävs ett stort antal referensprov för att täcka upp den förväntade variationen.

De kalibreringsmodeller som skapas utvärderas mot ett antal kriterier där robusthet och riktighet är primära kriterier. När kalibreringsmodeller utvärderas används ofta riktighet (accuracy) som kriterium. När det gäller biobränsle och i ännu högre grad avfall så är standardavvikelsen på referensvärdena relativt stora på grund av materialets heterogenitet så att riktighet i dess korrekta mening är svårt att bestämma, det "sanna" referensvärdet är okänt. I stället används RMSE(P), Root Mean Square Error (of Prediction), som är ett mått på hur väl modellens resultat överensstämmer med referensmetodens resultat. Genom att beräkna RMSEP och känna standardavvikelsen på referensmetoden kan ett metodfel beräknas.

Teoretiskt inom spektroskopi finns det ett linjärt samband mellan logaritmen på antalet absorberade fotoner och koncentrationen av det mätta materialet. I klassisk spektroskopi där ljuset passerar ett prov, ofta en vätska i en kyvett, kalibreras absorbansen vid en given våglängd med halten av materialet i kyvetten. I Optic-NIRS projektet har Reflektans Nära-Infraröd spektroskopi använts. Denna teknik skiljer sig på ett antal olika sätt mot klassisk spektroskopi vilket leder till att mer avancerade kalibreringsmetoder måste användas. En primär skillnad är att det kemiska fingeravtryck som ett NIR spektra utgör kan bestå av tusentalsöverlappande toppar, speciellt i ett i kemiskt hänseende så komplext material som biobränsle i form av skogsråvara.

De modeller som används till NIR är systemspecifika, det vill säga att de beror en kombination av den hårdvara som används och det kemiska system som skall mätas på. Inom ramen för projektet har ett antal lämpliga matematiska/statistiska metoder utvärderats i syfte att finna modeller som dels har en hög riktighet och precision, dels är robusta i en industriell miljö. De metoder som har studerats kan delas in i två huvudkategorier, dataförbehandlingar och regressionsmetoder. Förbehandlingar har till syfte att filtrera bort störningar, till exempel "scattereffekter" (ljusspridningseffekter) och att förstärka den del av signalen som är informationsbärande. De olika regressionsmetoderna har olika egenskaper till exempel hur de hanterar icke-linjära fenomen och hur robusta modellerna blir, vilket är viktigt i en industriell 24/7 situation. Olika förbehandlingar i kombination med olika regressionsmetoder har undersökts.

De förbehandlingar som undersökts är Standard Normal Variate (SNV), Multiplicative Scatter Correction (MSC), Savitzky-Golay derivator (SG) av olika ordningar och våglängdsselektionsmetoder. De regressionsmetoder som undersökts är Partial Least Squares (PLS), Artificial Neural Network (ANN), Gaussian Process Regression (GPR) och Support Vector Regression (SVR).

För bestämning av fukthalt på biobränsle visade det sig att en kombination av förbehandlingarna SNV+SG1 och regressions metoden GPR gav den lägsta

avvikelsen mellan referensanalyserna och de predikterade värdena både för intern validering och på ett externt test set. Avvikelsen uttryckt i RMSEV var 1.7 fukthaltsprocent.

På samma sätt undersöktes ett antal förbehandlingar och metoder för att med hjälp av HSI identifiera ett antal material såsom olika polymerer, trä och mat, primärt för att användas på kommunalt avfall.

Samma förbehandlingar av spektaldatan och dessutom Mean Centering (MC) som vid de kvantitativa modellerna undersöktes i kombination med ett antal metoder för materialidentifiering. Dessa metoder var, Radial Basis functions Neural Networks (RBNN), Support Vector Machine (SMV) och Discriminant Analysis PLS (PLS-DA). Bästa resultatet med avseende på både sensitivitet och specificitet erhöles med en kombination av SG1+MC med SVM.

Med traditionell NIR sensor kunde projektet visa att metodfelet på sensorn var lägre än felet för referensmetoden. Exempelvis för fukthalt där RMSEP beräknades till 2,2% och standardavvikelsen på ugnstorkning 1,8% leder till att NIR sensorn har ett metodfel på 1,3%, vilket kan anses som mycket gott. På samma sätt kunde det visas att NIR sensorn gav låga metodfel för askhalt och värmevärde (Övre Värmevärde).

HSI – Hyper Spectral Imaging visade sig vara en sensorteknik som kan skapa mycket värdefull information kring ett antal egenskaper på biobränslet. Data som HSI skapar är 3-dimensionell, till skillnad mot traditionell NIR som skapar ett spektrum, en vektor med data. HSI kan ses som en kamera som skapar ett antal monokroma bilder samtidigt, där varje bild är tagen vid en specifik våglängd, eller som en bild där varje pixel är ett NIR spektra. Där resultatet från traditionell NIR är genomsnittet av vad som passerat sensorn på bandet under en viss tid skapar istället HSI ett antal tidsdiskreta bilder från ett antal våglängder. Detta leder till att data från HSI kan analyseras både med hjälp av bildanalys metoder och med spektroskopiska metoder. Då varje pixel är ett spektrum kan varje pixel analyseras för kemiskt innehåll. Denna egenskap gör det möjligt att inte bara bestämma fukthalt osv. på varje flisbit utan också identifiera olika kemiskt annorlunda material, såsom plast, och även särskilja mellan olika plaster. En sådan analys av plaster har ej testats i detaljerat sätt inom projektet men skulle kunna vara mycket intressant för framtida arbeten. För avfallseldade kraftverk kan HSI bli ett kraftfullt verktyg för att i detalj kunna bestämma innehållet i avfallsbränsle.

När implementeringen av sensorsystemen vid Eskilstuna och Västerås utfördes så krävs också att sensorernas kalibreringar justeras för de faktiska förhållandena i anläggningarna. När NIR-sensorn är monterad över transportbandet sker en mätning under cirka 30 sekunder och den resulterande mätningen är ett medelvärde av det bränsle som passerat under den tiden. Från det bränsle som passerar tas ett stickprov på vilket referensanalys kan göras. Vid analys av fukt till exempel tas ett prov på cirka två liter från bandet. Detta prov analyseras sedan med standardmetoden torkning och vägning. Då bränslet är heterogent i sin natur så är det inte möjligt att få exakt analys av det som passerade under 30 sekunder, men genom att ta ett större antal sådana prover vid olika tidpunkter går det att med hjälp av statistiska metoder både kalibrera och validera sensorerna när de är

monterade on-line. För avfallsbränsle som är ännu mer heterogent än skogsbränsle användes ytterligare en metod för att validera sensorn. Genom att mäta fukthalt i rökgaserna och ta hänsyn till tidsförskjutningen mellan NIR mätning och rökgasmätning kunde NIR sensorns resultat valideras.

Sammantaget visade OptiC-NIRS projektet att det går att erhålla sensorresultat med god "riktighet" på transportbandet till pannan. Detta öppnar upp möjligheter till "feed-forward" styrning och tidig hantering av plötsliga förändringar av bränsleegenskaper såsom fukthalt på ett sätt som inte bara kan leda till bättre processekonomi utan också reducera mängden emissioner av icke önskade kemikalier.

Det finns ett antal intressanta kvarvarande frågeställningar kring dessa mjuka sensorer¹. Möjligheten att koppla och utnyttja denna sensorinformation till intelligent processtyrning, utveckla metoder för att utnyttja all den potential som HSI erbjuder, kanske extra intressant för avfallseldade kraftvärmeverk.

¹ P. Kadlec, B. Gabrys, S. Strandt (2009). *Data-driven Soft Sensors in the Process Industry*. *Computers and Chemical Engineering*. 33 (4): 795–814, doi:10.1016/j.compchemeng.2008.12.012.

Summary

Near InfraRed Spectroscopy (NIRS) offers rapid on-line analysis of biomass feedstocks and can be utilized for process control of biomass-based combined heat and power plants. Within the OPtiC-NIRS project we have carried out a full-scale on-site testing of different NIRS for online powerplant control at the facilities of Mälarenergi and Eskilstuna Strängnäs Energi och Miljö.

The project has been focused on developing and testing robust NIRS soft-sensors for fuel higher heating value and composition (incl. moisture, components such as recycle wood and glass, different type of plastics and ash) and combining them with dynamic models for on-line feed-forward process monitoring and control. Expected benefits include reduced risk of agglomeration and pollutant emissions formation as well as improved production control. A longer-term potential and ambition is to be able to identify the fossil content in municipal waste fuel, which can hopefully be addressed in a follow-up study.

Keywords

NIRS; Biomass; Waste; Combustion; Soft-sensors; Control.

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List of Abbreviations

ANN, Artificial Neural Network

ATEX, Equipment for potentially explosive atmospheres

CHP, Combined Heat and Power

DA-NIR, Diode Array Near Infrared

DCS, Distributed Control Systems

ERP, Enterprise resource planning

ESEM, Eskilstuna och Strängnäs Energi och Miljö

FFMPC, Feed-Forward Model Predictive Control

FT-IR, Fourier Transform InfraRed

FT-NIR, Fourier Transform Near InfraRed

GPR, Gaussian Process Regression

HDPE, High Density PolyEthylene

HS, HyperSpectral

HSI, HyperSpectral Imaging

HSI-NIR, HyperSpectral Imaging in the Near InfraRed Region

K, Kelvin

KNN, K-Nearest Neighbor

LDPE, Low Density PolyEthylene

MC, Moisture Content

MC%, Moisture Content in percentage by weight

MSC, Multiplicative Scatter Correction

MSW, Municipal Solid Waste

NIR, Near InfraRed (850-2500nm, 4000–12000 cm⁻¹)

NIRS, Near InfraRed Spectroscopy

PC1, Principal Component 1, from PCA/PLS

PCA, Principal Component Regression

PET, Polyethylene terephthalate

PLS, Partial Least Squares

PLS-DA, Partial Least Squares Discriminant Analysis

PLSR, Partial Least Squares Regression

PP, PolyPropylene

PS, PolyStyrene

PVC, PolyVinyl Chloride

RBNN, Radial Basis functions Neural Networks

RDF, Refuse-Derived Fuel

RGB, Red, Green and Blue

RMSE, Root Mean Standard Error

RMSECV, Root Mean Standard Error calculated from CrossValidation samples

RMSEP, Root Mean Standard Error of Prediction

RMSEV, Root Mean Standard Error calculated from Validation samples

ROI, Region Of Interest

SCADA, Supervisory Control And Data Acquisition

SG, Savitzky-Golay filtering

SG1, 1st derivative using Savitzky-Golay filtering

SG2, 2nd derivative using Savitzky-Golay filtering

SGS, ? In HSI plastics part

SME, Small and Medium size Enterprises

SNV, Standard Normal Variate

SV, Supported Vector

SVM, Support Vector Machines

SVR, Support Vector Regression

TCP, Transmission Control Protocol

UDP, User Datagram Protocol

wt%, percentage by weight

1 Introduction

The OptiC-NIRS project focuses on the development and demonstration of NIRS soft-sensors for fuel characterization (biomass and waste). Soft sensors are widely used to estimate process variables that are difficult to measure online. Soft sensor is a common name for software where several measurements are processed together. In the case of NIR, absorption from several wavelengths is measured simultaneously and correlated to properties of the measured material. These soft-sensors are key technological bricks in enabling feed-forward model-predictive control of biomass- and waste-fired combined heat and power plants. This control concept enables improved control of circulating fluidized bed and bubbling bed boiler systems by utilizing feed-forward information from characterizing in the coming feedstock, be it biomass or refused-derived fuel (RDF). The approach is illustrated in Figure 1.

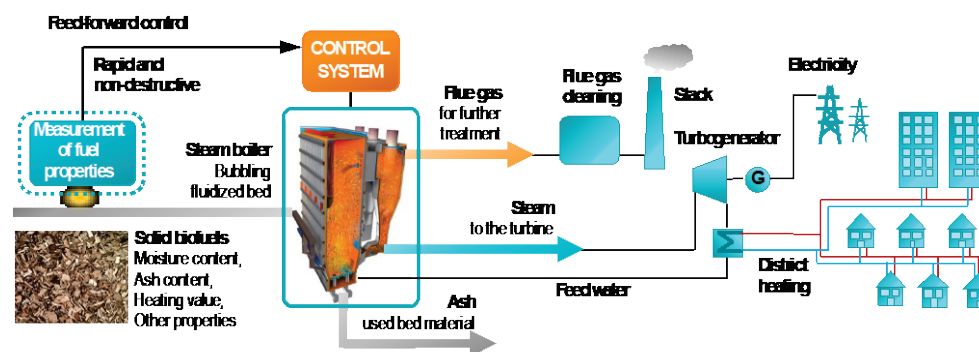


Figure 1: Illustration of the approach employed within the OptiC-NIRS project

Some of the benefits of the approach relate to maintaining a more stable bed and riser temperature², reducing agglomeration and the potential for corrosion as well as enabling diagnostics in relation to the need for sand renewal.

Previous work has shown that it is possible to determine the moisture content in biofuel, even when it is transported on a conveyor belt³. Further research has shown that the NIR method is capable of determining moisture content in a wide variety of different parts from the forest industry, such as woodchip, bark, sawdust, GROT and used wood chips with good conformity with the reference method^{4,5}. Furthermore, it has been shown that it is possible to measure biofuel from wood, transported in a feed screw and that feed-forward control of the bed

² The main body of the boiler is assumed to comprise a lower part, the bed, and an upper part, the riser where the evaporators are typically located (see Figure 39). It is assumed that the vast majority of the combustion takes place in the bed, while only some residual combustion may take place at the riser.

³ Jenny Nyström, Lars Axrup, Erik Dahlquist. (2002) *Långtidsutvärdering av nya on-line fukthaltsmätare för biobränsle*. Värmeforsk Rapport 2002:763

⁴ Magnus Berg, Sven Erik Wiklund, Mikael Karlsson, Robert Tryzell (2005) *Automatisk fukthaltsbestämning av biobränslen med NIR-metoden*. Värmeforsk Rapport 2005:935

⁵ Erik Dahlquist, Lars Axrup, Jenny Nyström, Eva Thorin, Ana de la Paz. (2005) *Automatisk fukthaltsmätning på biobränslen med NIR samt radiofrekvent spektroskopi*. Värmeforsk Rapport 2005:936

temperature could be possible⁶. Investigations has been made about the possibility to use the determined moisture content to stabilize the bed temperature. Results has been promising when using manual adjustments, but time and conditions did not lead to any conclusive results using MPC⁷. Furthermore, none of the earlier works has focused on refuse derived fuel, which can have complicated composition as illustrated through Figure 2. Refuse derived fuel is differentiated to municipal solid waste; in the latter the organic matter part ranges between 50% and 60%, with plastics and paper/cardboard in the range of 10% and 15% respectively⁸.

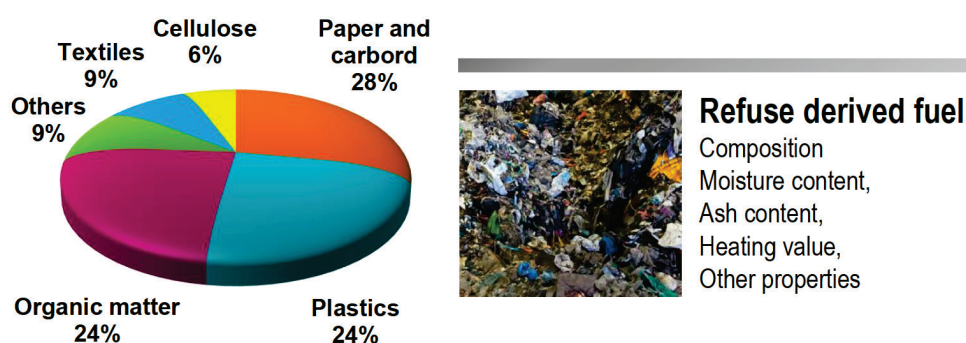


Figure 2: Refuse derived fuel composition and properties of interest

Within the project new soft-sensors have therefore been developed using a variety of approaches ranging from traditional FT-NIR and DA-NIR to Hyperspectral NIR imaging; even Raman NIR spectroscopy using 2 different laser systems was investigated but has shown to be inappropriate for the specific application. The most promising techniques have been implemented and demonstrated on-line at Mälarenergi, in Västerås, Sweden, and at Eskilstuna Strängnäs Energi och Miljö, in Eskilstuna, Sweden, for RDF and woody biomass fuels, respectively. The sensors provide the feed-forward information required by developed dynamic models, coupled for the purposes of advanced diagnostics and model-predictive control.

The report is written with future users (CHP plant operators) and developers (commercialisation partners, SMEs) of NIRS technology as the audience in mind. The lab-scale experiments are presented in detail in Section 2, while the full-scale demonstrations are described in Section 3. The work is concluded in Section 4 where detailed lessons learned are presented along with a future outlook. A retrospective look at the OptiC-NIRS objectives and the extend these have been achieved is given in Appendix A while a list of publications produced is provided in Appendix B.

⁶ Torbjörn Lestander, Björn Hedman, Jonas Funkqvist, Andreas Lennartsson, Marcus Svanberg. (2008) *On-line NIR-fukthaltsmätning för styrning av panna i värmekraftverk*. Värmeforsk Rapport 2008:1059

⁷ Anders Avelin, Erik Dahlquist, Per-Erik Modén. (2008) *Forskning kring pannstyrning med on-line fukthaltsmätning på biobränsle*. Värmeforsk Rapport 2008:1073

⁸ C. Montejo, C. Costa, P. Ramos, M.D.C.Márquez. (2011). *Analysis and comparison of municipal solid waste and reject fraction as fuels for incineration plants*. Applied Thermal Engineering, 31: 2135-2140.

2 Lab-scale Experiments

NIR spectroscopy is among the most popular techniques for developing soft-sensors for characterizing in real-time incoming feedstocks. A detailed review of different applications of soft-sensor technology as applied to biomass conversion process is provided in ⁹.

Within the Optic-NIRS project, NIRS calibrations have been developed and further improved at the SPECTRA lab of the Future Energy Center at Mälardalen University, using a number of NIRS instruments available.

The lab-scale work begun by selecting those parameters that were most important for boiler performance. Following several consultations with the project's industrial partners, as well as the identified gaps in the literature, moisture and ash content as well as higher heating value were selected. In the subsections below, the lab-scale developments based on traditional NIRS as well as on hyperspectral imaging are presented in detail. The respective arrangements are show in Figure 3 and Figure 4.

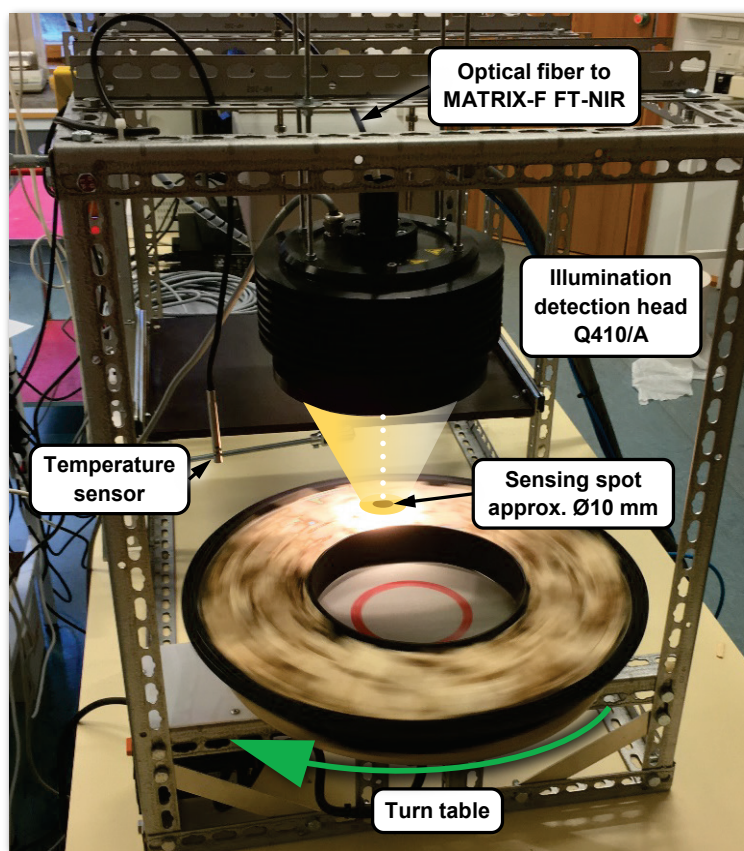


Figure 3: Description of traditional NIRS system on a turntable

⁹ Jan Skvaril, Konstantinos Kyprianidis, Erik Dahlquist. (2017) *Applications of Near Infrared Spectroscopy (NIRS) in Biomass Energy Conversion Processes: A Review*. Applied Spectroscopy Reviews.

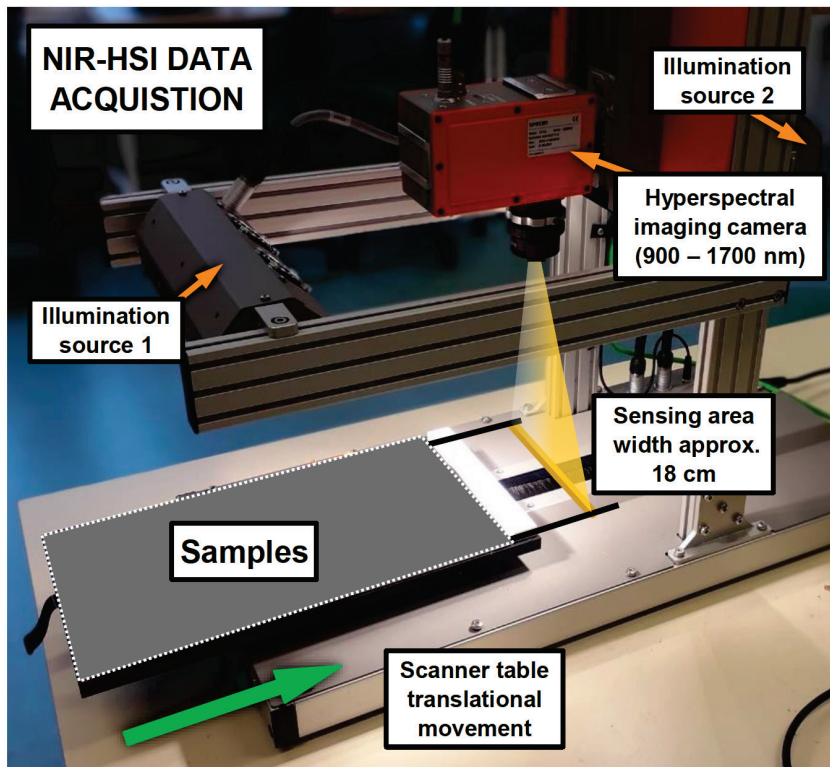
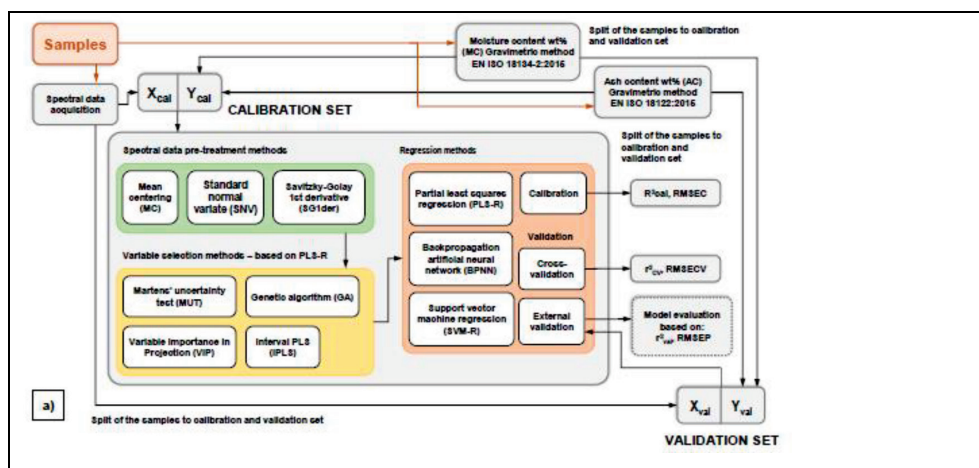


Figure 4: Description of HSI system

The multivariate data analysis workflow is illustrated in Figure 5 and is explained in detail in the following subsections.



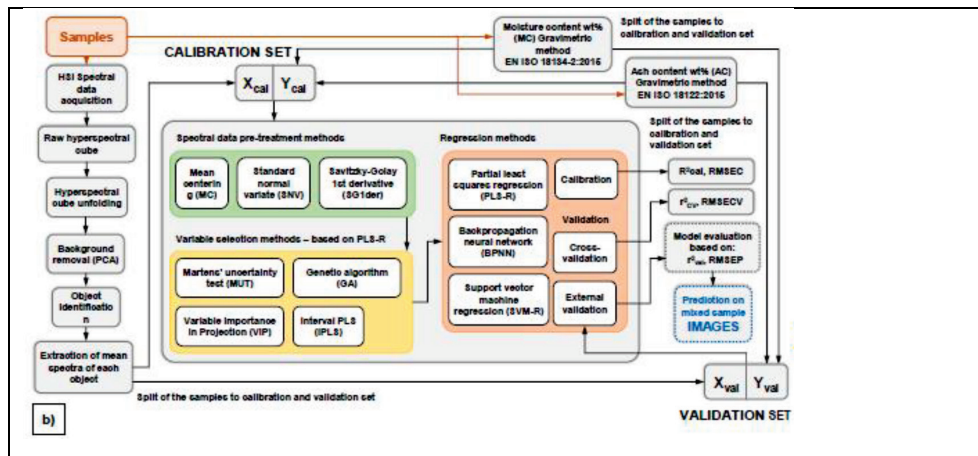


Figure 5: Schematic illustration of calibration approach: a) Traditional NIRS system; b) HSI system

TRADITIONAL NIR SPECTROSCOPY

Using traditional chemometrics methods (PCA/PLS), a set of initial calibrations for the afore-mentioned parameters was developed, based on a Bruker FT-NIR system, which is a traditional spectrophotometer. A turntable has been used for regulating the speed of the sample. A large number of fuel samples was tested in the lab using reference methods, scanned using the NIR system and fed to the chemometric algorithm for developing the calibrations. For details on the underlying testing and chemometrics methods for developing such calibrations, the interested reader is referred to ¹⁰. The range of validity for these calibrations is shown in Figure 6, along with key statistical figures of merit.

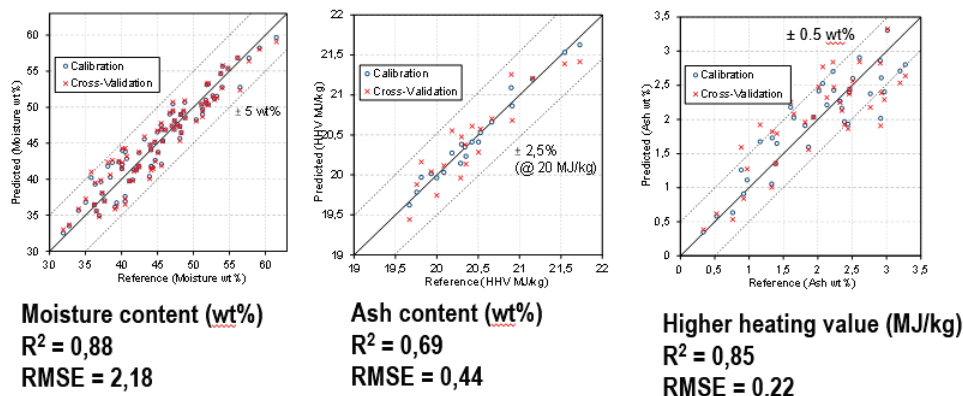


Figure 6: Range of validity for traditional NIRS calibrations

In order to validate the fit between predicted values and reference values the RMSE(P) (Root Mean Square Error (of Prediction)) is used. RMSEP shall be seen as

¹⁰ Olivia Winn, Kiran Thekkemadathil Sivaram, Ioanna Aslanidou, Jan Skvaril, Konstantinos Kyprianidis. (2017) *Near-infrared spectral measurements and multivariate analysis for predicting glass contamination of refuse-derived fuel*. Elsevier. Energy Procedia, 142: 943-949.

an equivalent to standard deviation but over a range and not only at one single expected value. The unit for RMSEP is the same as for the measured variable, just as for standard deviation.

Equation 1: RMSEP definition

$$RMSEP = \sqrt{\frac{\sum_{i=1}^n (y_{i,pred} - y_{i,ref})^2}{n}}$$

RMSEP is insensitive for the size of the range and can directly be compared to standard deviation on lab. It's not uncommon to use R2 to account for how well predicted values correspond to reference values, but R2 should be interpreted with caution since it is range dependent. Given that two set of data can show different R2 values but the same RMSEP if the ranges are different.

If the RMSEP and the STD for the reference analysis are known the error of the method can be determined since the RMSEP is the sum of the error in the method and the error in the method.

Equation 2: Estimated Error Method

$$Estimated\ Error\ Method = \sqrt{RMSEP^2 - STD_{ref}^2}$$

When looking at the presented model for moisture for example, "true" moisture content is not known and the reference method is not magnitudes more accurate than the NIR-method and hence the accuracy of the method can't be determined, however the error of the method can be estimated.

When using the standard "SS-EN ISO 18134-2:2015" for determining moisture content in solid biofuel it is commonly reported that the method have a STD of 1.5 – 1.8%. The RMSE for the prediction is 2.2%, inserting those numbers in Equation 2 give a method error of 1.3 – 1.6%. Which conclude that the NIR method have better accuracy than the reference method in this case.

In the next step, a process was developed to improve the initial calibrations to the accuracy required for a full-scale demonstration. Several advanced post-processing techniques have been considered, including Support Vector Machines, Gaussian Process Regression and Artificial Neural Networks. The full workflow for the calibration model optimization is shown in Figure 7. The application of the method is covered below only for the case of moisture, but it is equally applicable to other measured quantities such as fuel heating value and ash content.

Prior to applying these post-processing techniques as it is important to pre-treat the underlying raw data in the best way possible. A number of techniques have been explored in this case, from Standard Normal Variate to considering 1st and 2nd derivatives, after applying Savitzky–Golay filter (a polynomial approximation). The resulting signals starting from the raw spectra are illustrated in Figure 8.

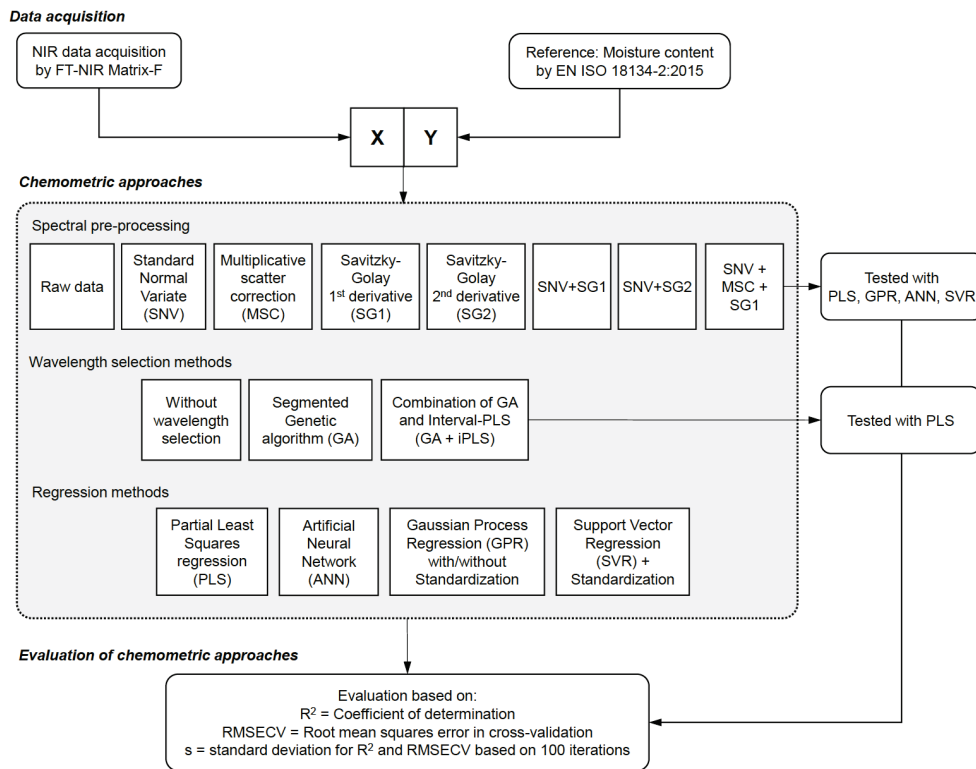


Figure 7: Chemometric approach employed with traditional NIRS system

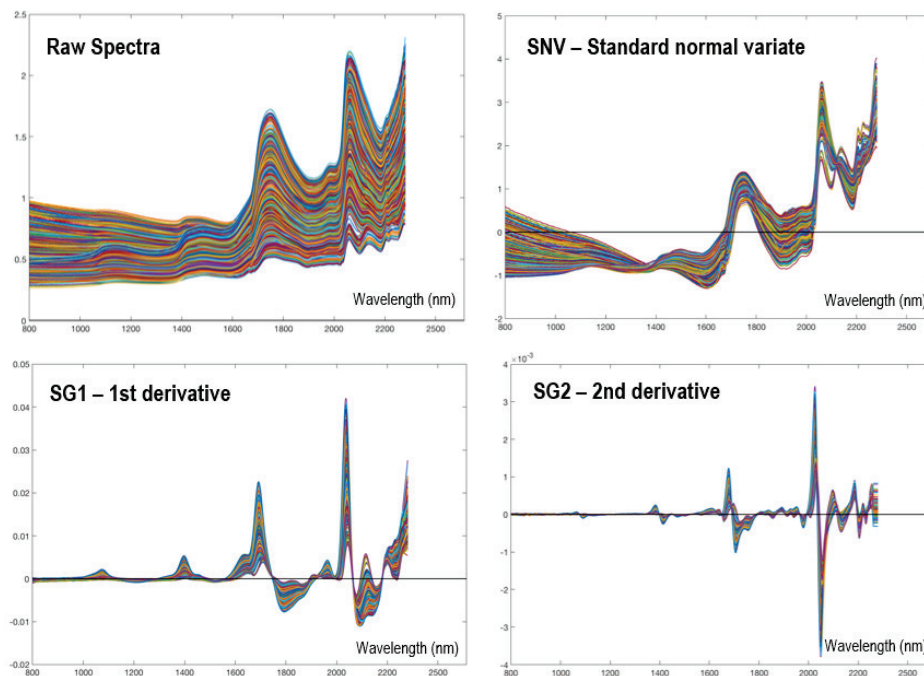


Figure 8: Raw spectra from traditional NIRS and effect of different pre-treatment techniques

From an optimal calibration point of view the optimization problem needs to consider the different pre-processing and post-processing techniques at the same time. The resulting analysis should therefore look at optimal pairs of pre- and post-processing techniques and different fitting metrics like R^2 and RMSECV. A summary of the different combinations that were explored following the presented full workflow is given in Table 1 focusing on the selected statical figures of merit, for the case of moisture content. As can be seen the combination of SNV and SG 1st derivative for data pre-treatment gave the most promising results on the training data set.

Table 1: Summary of results from different optimized combinatorial methods

Dataset	PLS		GPR		ANN		SVR	
	R^2	RMSECV	R^2	RMSECV	R^2	RMSECV	R^2	RMSECV
Raw data	0.97	2.73	0.95	3.0	0.93	2.31	0.94	2.47
SNV	0.98	2.41	0.98	2.0	0.98	2.16	0.97	2.14
MSC	0.98	2.46	0.97	2.01	0.98	2.32	0.97	2.15
SG1	0.97	2.75	0.97	2.23	0.98	2.42	0.97	2.17
SG2	0.97	2.88	0.96	2.19	0.97	2.67	0.96	2.24
SNV+SG1	0.98	2.31	0.98	2.03	0.98	2.26	0.98	2.04
MSC+SG2	0.98	2.36	0.98	2.04	0.98	2.34	0.98	2.03

Whilst the methods were checked first on the training data set, the ultimate measure of quality on the results derived arrives from testing the calibration on independent data, that were not used in the calibration derivation. The latter is known as test set, in this case it is RMSEV along with R^2 that is the important fitting metric. This calibration optimization approach gave very good results as shown in Table 2, with GPR being the most promising technique, but the rest also being considerably accurate.

Table 2: Results for the best combinations of pre-processing and calibration techniques

Dataset	R^2	RMSEV
SNV+SG1+PLS	0.98	2.31
SNV+SG1+GPR	0.98	1.69
SNV+ANN	0.98	2.01
SNV+SG1+SVR	0.98	1.96

A further step for improving NIR calibrations is that of wavelength selection, as opposed to using the entire NIR spectra acquired. Within the project various methods were tested and evaluated while using PLS regression method. The aim was to minimize the number of wavelengths/intervals used and improve the overall prediction accuracy of the calibration. As shown in Figure 9 the selected wavelengths mostly correspond with the absorption bands arising from vibrational transitions of H-O-H molecule, in the case of moisture. This includes a combination of symmetric and asymmetric stretching and bending vibrations.

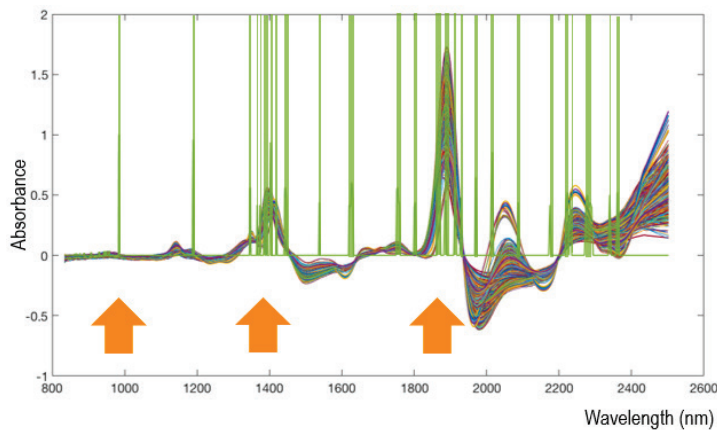


Figure 9: Peaks in specific wavelengths due to moisture content

The overall improvement achieved in the NIR spectra calibrations is summarized through Figure 10 and Table 3. For key parameters an improvement of over 33% in prediction accuracy (RMSEP) was achieved.

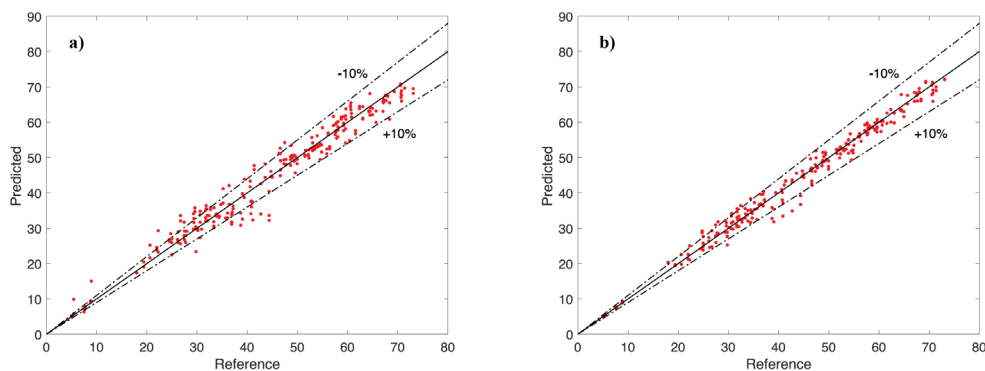


Figure 10: Resulting parity plots on test data using GPR: a) Best prediction using raw dataset; b) Best prediction with selected wavelengths from pre-process

Table 3: Figure of merit overall improvement achieved for the NIR spectra calibrations

Model	Execution time for prediction of one sample (ms)	Pre-treatment	Selection of variables	R ²	RMSEP (wt%)
PLS (reference model)	4.99	MSC	Full NIR region	0.96	2.46
GPR	9.15	SNV +SG1	Full NIR region	0.98	1.69
GPR + wavelength selection	4.97	SNV +SG1	GA (71 selected)	0.98	1.64

➔ **Approx. 33% improvement in prediction**

Overall, and in relation to the project aims, it was concluded that trying to keep a constant sample-to-sensor distance to maintain focus is possible. It can be successfully achieved through the design and construction of an appropriate instrument holder (see also later sections), albeit this is far from a trivial task.

It was possible to develop lab-scale NIRS calibration models with a fit between predicted values and reference values well within a couple of % units (after model optimization process) for both moisture content and higher heating value. Ash content was more challenging but fit between prediction and reference within 0.5% were shown to be possible. It can also be concluded that the employment of less traditional machine learning techniques (such as GPR, instead of PLS) has led to significant improvements in models. Nonetheless, NIRS prediction models will need to be improved continuously through re-training/validating the algorithm by adding new reference/spectral data, particularly when the model is running on-line with real time data. The raw material for biofuel does not only have reasonable variation but can also exhibit variation from one year to another, beyond that new suppliers can deliver material with various composition. Hence is a dynamic strategy for automatic updating models an important part of a long-term use of NIR as sensor.

HYPERSPECTRAL NIR IMAGING

Further to the so-called traditional NIR measurement technique discussed in the previous sub-section, the hyperspectral imaging (HSI) technique was also utilized within the OptiC-NIRS project. A dedicated HSI-NIR camera (from Specim) was utilised for this purpose. The measurement technique as well as the selected instrument are shown in Figure 11.

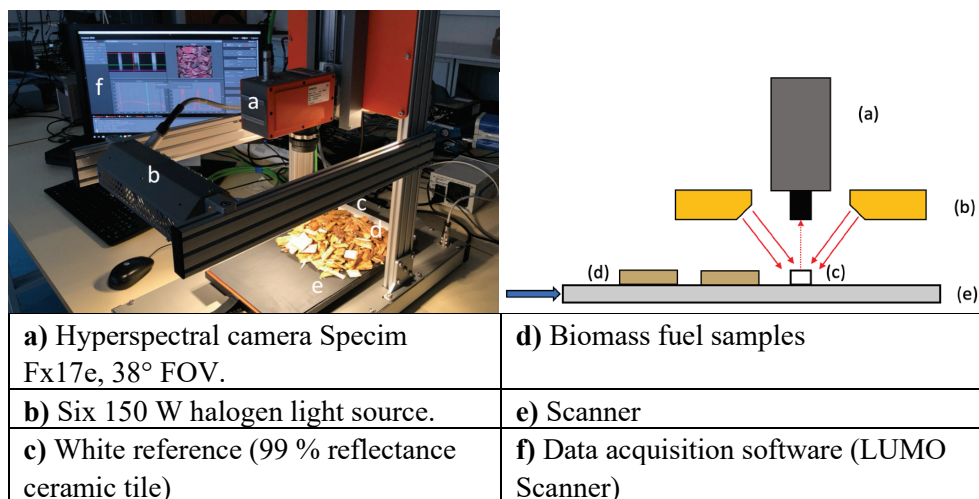


Figure 11: Measurement technique and HSI instrument

Both traditional NIR and HSI produce spectral information in the NIR spectral region. The traditional NIR relies on measuring on a surface, typically 95% of the energy on a circle with 5 cm diameter, however the measurement is taken over a time period (30 sec) and since the conveyer band is moving the resulting measurement is done as an average of a “band” with a width of 5 cm and a length depending on the speed of the conveyer belt. The present HSI system is simultaneously measuring a 640 pixels long array, where each pixel is a NIR

spectra from the material at that point. Resulting in a matrix of data. The HSI works as a high-speed camera with a frame rate of several hundred per second, so when the conveyer belt has moved the material a short distance a new array of spectral pixels is measured. After a number of measured arrays, a 3D picture is obtained. The obtained hyperspectral cube (a tensor of data) decomposition is shown through Figure 12 for wood chips.

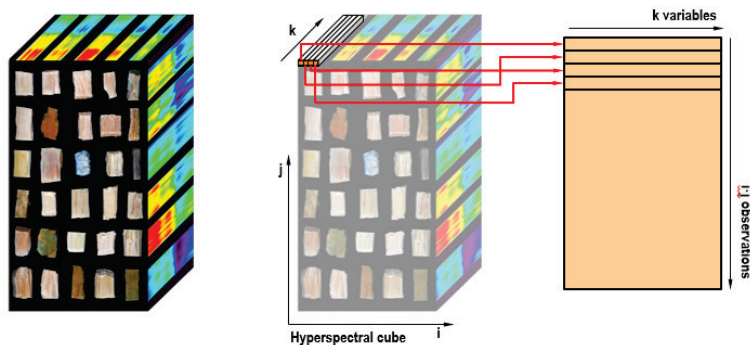


Figure 12: The hyperspectral cube produced by the HSI instrument

It can in essence be described as a vast number of pictures on top of each other, where each picture is a monochrome representation of the material in a certain wavelength. It can also be described as a picture that for each pixel has a 3rd dimension represented as a NIR spectra from that pixel, as illustrated through Figure 13.

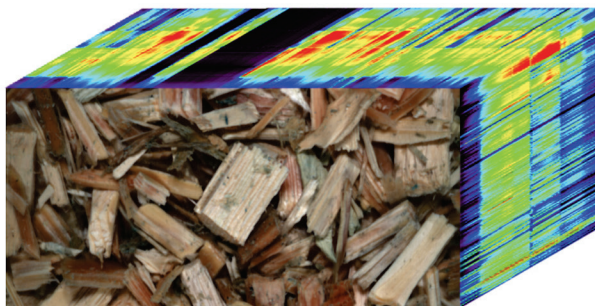


Figure 13: 3-dimensional picture produced by the HSI instrument

Differences between the raw reflectance of wood chips and bark present in the same sample are shown in Figure 14. Wood chips and bark have a different chemical composition and often contain different moisture levels. In the picture below it can be seen that the area measured on the square with bark have a heterogeneous look which also is manifested in the spectra from those pixels, at the same way the square with wood chips contains different wood chips with slightly different chemical composition and hence the spectra differ more. The bigger span in reflectance values also depend on scatter effects since the material in the wood

chips square have different angles to the light source and detector, i.e., also more heterogeneous physical properties.

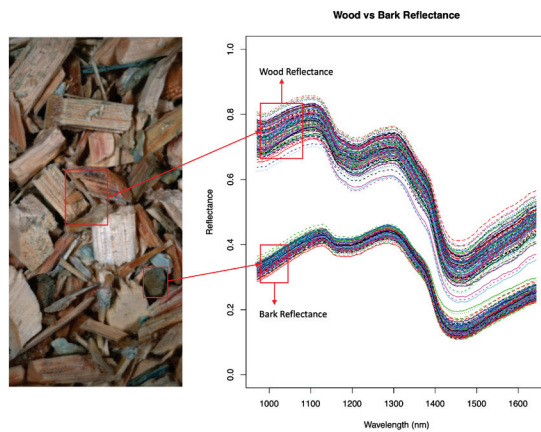


Figure 14: Differences between the raw reflectance of wood chips and bark

When taking images for the purpose of building a soft-sensor calibration, some of the spectral data at the start and end of the spectrum had to be removed due to high level of noise. Mean centering was first applied, then PCA was applied to the HSI image to reduce the size of the image and to extract only the useful information. Then a new image was constructed using PC1 since it gave the highest variance. Background subtraction was performed by putting a threshold with reflectance less than 0.1. To have more flexibility on the hypercube image, a model was created to select the region of interest (ROI) manually. This enabled the developed calibration to detect the difference between the spectra of bark and that of wood chips. The process is illustrated in Figure 15.

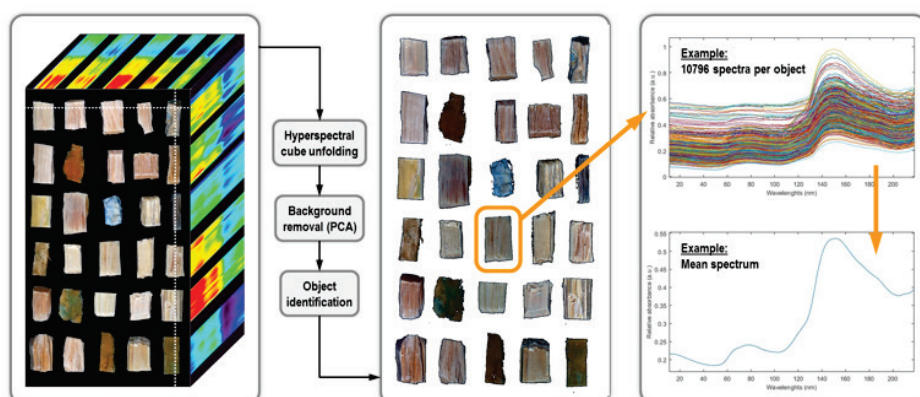


Figure 15: Process for developing calibrations for HSI instrument

Several pre- processing techniques have been tested within this project. In this case Savitzky-Golay 1st derivative (SG₁) and SNV-Detrend method gave the best result.

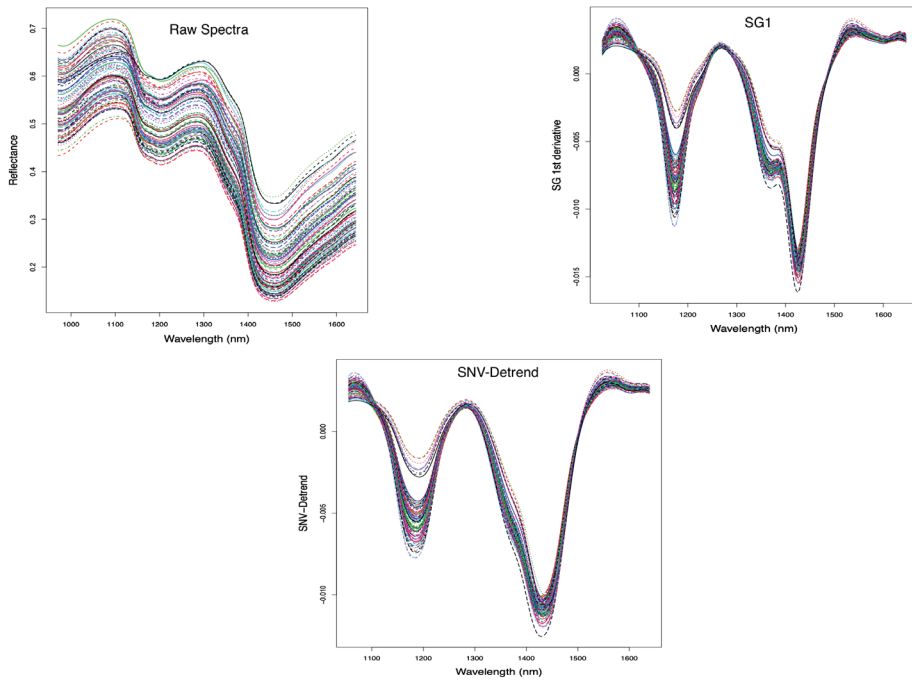


Figure 16: Comparison of pre-processing techniques for HSI spectra

In the raw spectra illustrated through Figure 16 there is a dip in spectra around 1450 nm and this is due to O-H overtone. Another dip is seen around 1190 nm, representing the reflectance bands of C-H stretching second overtone, which is related to the high-energy vapor phase of the samples.

Once the hypercube image has been properly treated and pre-processed it was used to build the calibration models. For this step, a number of approaches were considered, from using Partial Least Squares (PLS), to Support Vector (SV), K-Nearest Neighbor (KNN), and Artificial Neural Network (ANN). The approach to training the ANN is shown in Figure 17.

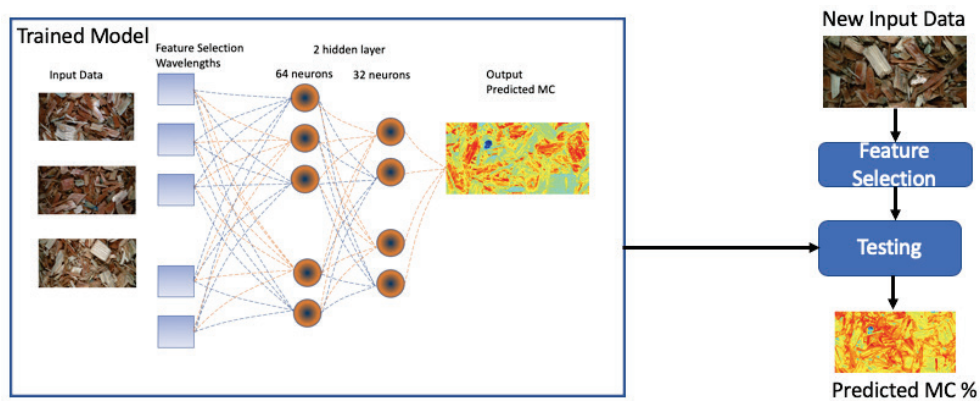


Figure 17: Training approach of ANN from HSI spectra

The cross-validation method was employed since the number of samples (100 for training and 10 for testing) are small. It was noticed that PLSR and ANN model with SG₁ spectra treatment gave the best result for predicting moisture content in the samples taken. This is evident from Table 4 and Figure 18 that summarize the performance on the selected statistical figures of merit for the different methods applied for predicting moisture content. It can be noted that the KNN method gave the least reliable results.

Table 4: Summary of cross-validation results for different methods predicting moisture content

PLS Regression Statistics						SVR Regression				
Treatment	LVs	R2_cal	RMSEC	R2_CV	RMSECV	Treatment	R2_cal	RMSEC	R2_CV	RMSECV
Raw	7	0.958	1.345	0.9476	1.503	Raw	0.931	1.7275	0.918	1.8789
SG1	7	0.9658	1.213	0.955	1.391	SG1	0.9516	1.4661	0.9361	1.6826
SNV- Detrend	7	0.9607	1.301	0.9504	1.462	SNV- Detrend	0.9506	1.4744	0.9347	1.6972
KNN Regression, K = 9						ANN Regression				
Treatment	R2_cal	RMSEC	R2_CV	RMSECV	Treatment	R2_cal	RMSEC	R2_CV	RMSECV	
Raw	0.9302	1.4246	0.86213	2.4347	Raw	0.9594	1.5575	0.8963	1.7524	
SG1	0.9425	1.9682	0.8752	2.2854	SG1	0.9439	1.5934	0.9124	1.6259	
SNV- Detrend	0.9352	1.4105	0.8652	2.3541	SNV- Detrend	0.9518	1.458	0.9152	1.5899	

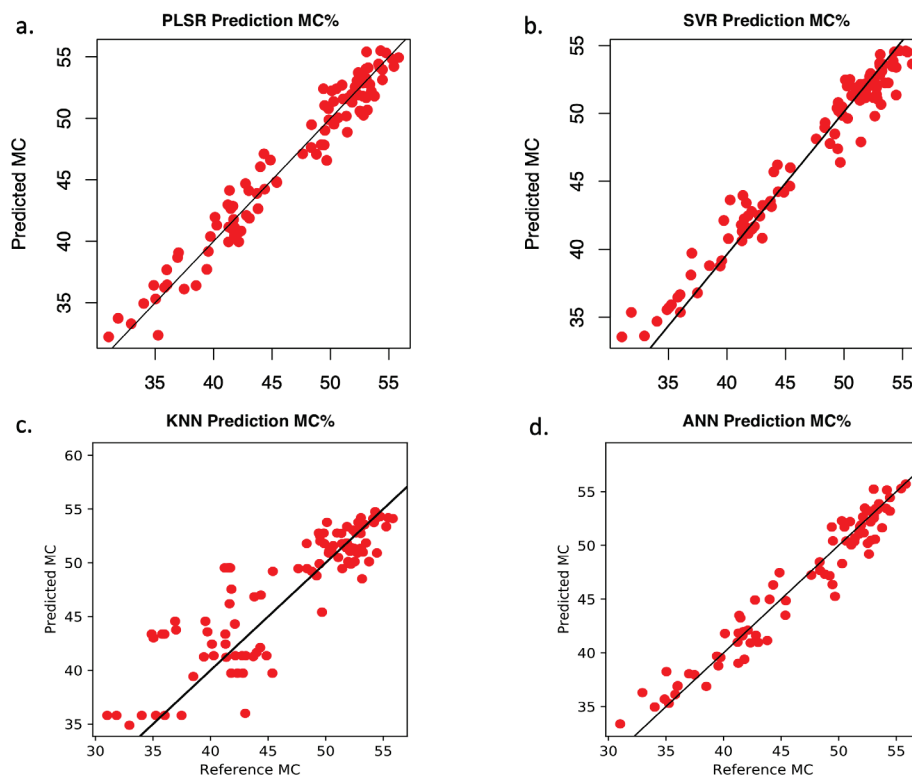


Figure 18: Parity plots for different methods predicting moisture content

Further to using the R2 and RMSECV metrics to judge the quality of the regression, just as with FT-NIR, cross-validation and independent test sets were considered.

As can be seen in Table 5 - and taking into account the error in the reference analysis - no significant differences can be seen between the tested methods. KNN did not show promising results and hence has not be included in the table.

Table 5: Summary of independent test set results for most promising prediction combinatorial methods

Model	RMSEP	R ²
PLSR-SG1	1.537	0.9247
SVR-SG1	1.5982	0.9189
ANN-SG1	1.6185	0.9174

In a final step, the best model was fitted to all the test samples to predict the moisture content on pixel basis of the hypercube. The results for this type of calibration are shown through Figure 19 in the form of an RGB picture with the color scale indicating moisture content. The approach was consequently applied for predicting ash content as well as shown through Figure 20.

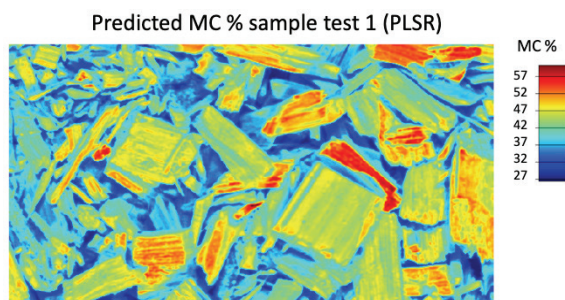


Figure 19: Moisture content prediction as an RGB image

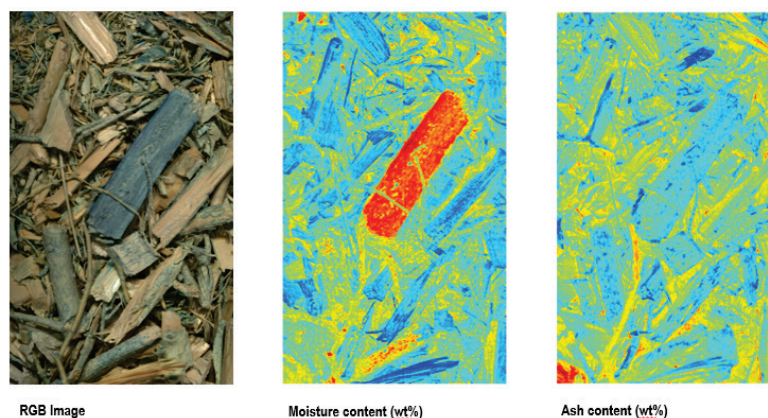


Figure 20: Comparison of raw RGB picture vs moisture content and ash prediction RGB pictures

The HSI system was also used for analyzing a number of other materials typically found in municipal waste. Average NIR spectra of materials included in this study acquired by the HSI camera and extracted from the hyperspectral cube are shown

in Figure 21. Results obtained from the identification of organic polymers (i.e. plastics) by using the FT-IR spectrometer available at the SPECTRA lab revealed that samples in each group contained various amounts of plasticizers and other additives making the classification challenging. Results of subsequent classification modelling showed that data pre-processing had significant impact on resulting accuracy of classification models.

The pre-processing techniques or combinations being the most (in green) and the least (in red) successful in classification are shown in Table 6. The accuracy is expressed as average of sensitivities calculated for all of the classes. PLS-DA reached overall the lowest accuracy. SVM reached the highest accuracy of 94 % for combined pre-processing by Savitzky-Golay 1st derivative and mean centering.

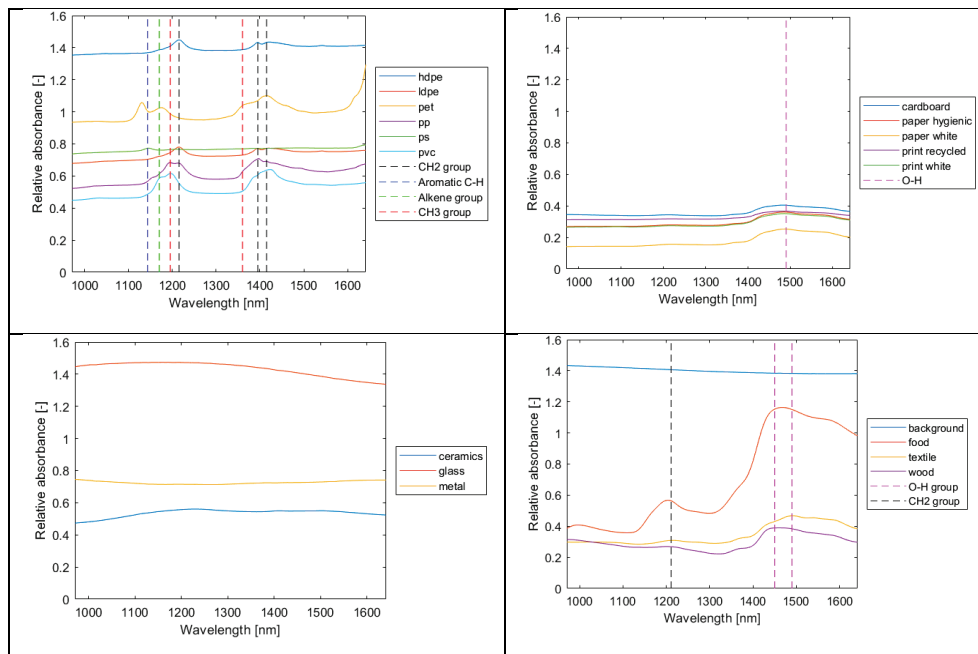


Figure 21: Average NIR spectra extracted from HSI data for different materials

Table 6: Classification results for different pre-processing techniques and methods

Pre-processing method	PLS-DA	SVM	RBNN
No pre-processing	64%	-	90.6%
SGS	64.3%	-	90.4%
SGS + mean centering	74.7%	92.4%	89.9%
SGS + SNV	88%	92.6%	89.6%
SGS + 1 st derivative	85.1%	93.8%	90.7%
SGS + 1 st derivative + mean centering	85.8%	94%	90.3%
SGS + 1 st derivative + SNV	83.2%	91.5%	88.3%
SGS + 2 nd derivative	84.4%	91.1%	88.8%
SGS + 2 nd derivative + mean centering	84.9%	91.5%	88.6%
SGS + 2 nd derivative + SNV	82.9%	87.2%	81.8%

The best pre-processing techniques of highest overall accuracy for each of the classification methods were selected from this evaluation above and the classification results were analyzed in more detail. The results shown in Table 7 focus on sensitivity, specificity and classification confusion, derived from the confusion matrix, for three developed classification models. Generally, the lowest sensitivity was achieved for incombustibles and PS. Most common misclassifications are done for incombustibles being confused with the background and for PS being confused with incombustible materials and background.

Table 7: Sensitivity, specificity and classification confusion for different models

Class	PLS-DA			SVM			RBNN		
	Sensitivity	1 - Specificity	Most confused with	Sensitivity	1 - Specificity	Most confused with	Sensitivity	1 - Specificity	Most confused with
Backgr.	88.3%	4.0%	incombustibles	97.8%	2.2%	-	98.9%	4.0%	-
Paper	74.3%	0.3%	textile	97.5%	0.5%	-	95.0%	1.3%	-
Incomb.	60.9%	2.5%	background	78.7%	3.0%	background	64.4%	1.8%	background
Food	98.4%	1.6%	-	98.7%	0.0%	-	96.4%	0.0%	-
PE	89.5%	0.2%	-	86.0%	0.2%	incombustibles	85.3%	0.1%	-
PET	97.3%	0.1%	-	94.5%	0.0%	-	91.6%	0.0%	background
PP	90.4%	0.5%	incombustibles	95.1%	0.1%	-	92.2%	0.2%	-
PS	73.7%	0.4%	incombustibles	85.0%	1.0%	incombustibles	86.0%	2.6%	background
PVC	99.2%	0.1%	-	97.9%	0.0%	-	95.2%	0.0%	-
Textile	97.8%	2.1%	-	97.8%	0.1%	-	94.7%	0.3%	-
Wood	98.2%	1.3%	-	98.2%	0.1%	-	97.9%	0.0%	-

The models were further externally validated, using HSI spectral acquired from separate validation mixtures. The prediction was done by classifying each pixel of the acquired hyperspectral image. The accuracy of classification during external validation was evaluated for four different pre-processing methods. Furthermore, demand on computational time was measured as the time needed for each model to classify approx. 1.5 million pixels (i.e. data points) of acquired hyperspectral images. The least demanding model on computational time was PLS-DA, followed by RBNN, requiring approx. 10 times more time, and the most computationally demanding model was SVM, requiring approx. 100 times more time than PLS-DA.

Results of the prediction are shown in Figure 22, Figure 23, and Figure 24 where different reference color of each pixel represents a predicted class. Figure 22 presents classification predictions by the PLS-DA model, Figure 23 presents results for the SVM model, and Figure 24 for the RBNN model. The results are shown as RGB pictures and are based on predictions using the best performing pre-processing technique i.e., SG1 + MC. The tables embedded within these figures present results for each material class.

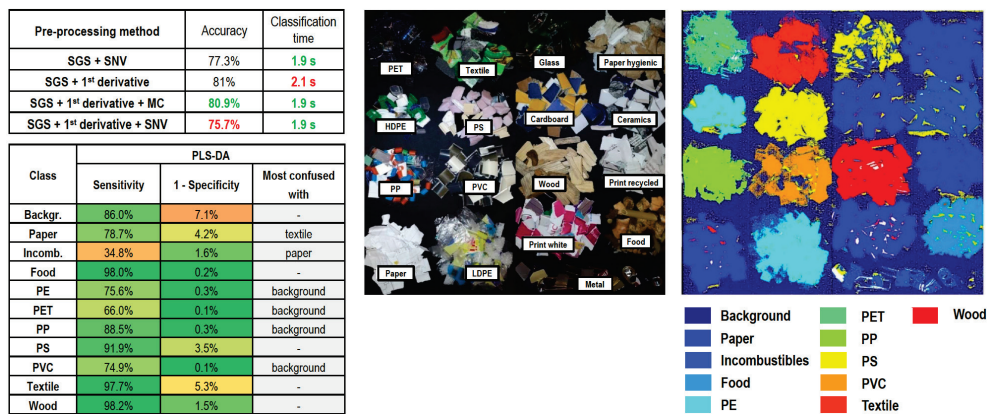


Figure 22: Classification predictions using the PLS-DA model (external validation set)

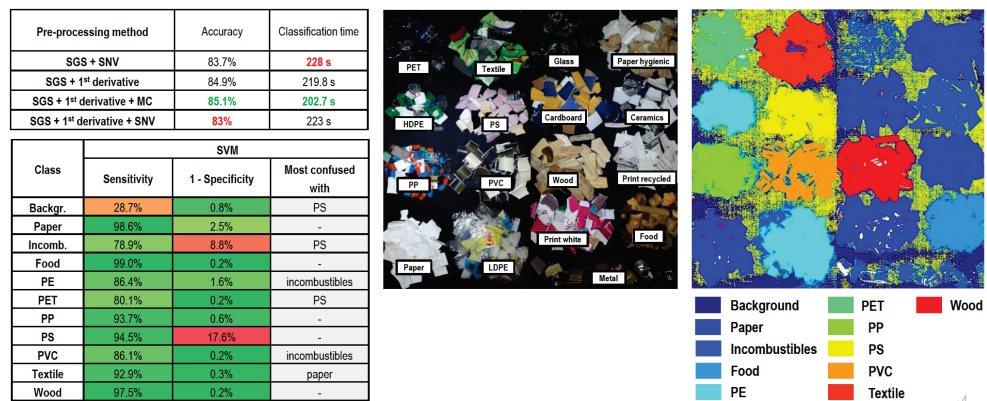


Figure 23: Classification predictions using the SVM model (external validation set)

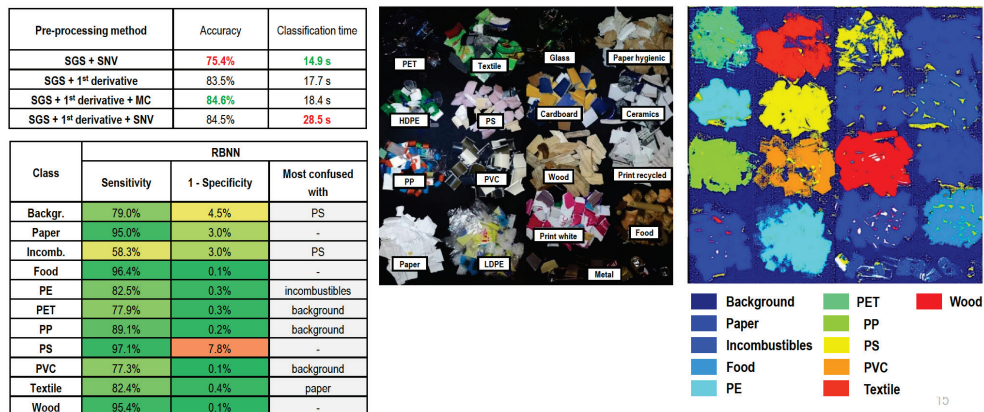


Figure 24: Classification predictions using the RBNN model (external validation set)

Generally, the best sensitivity was achieved for food, PS, and wood. Nevertheless, models often struggled with correct classification of incombustible materials. Overall, best results were reached for SVM, even though the model had a very low sensitivity in background identification. Confusions between background and PS can be largely explained by their very flat spectral profiles in the given spectral range. It is shown that consistency of classification by PLS-DA throughout the pile was lower compared to RBNN. Furthermore, when classifying by SVM a large part of the background was classified as polystyrene.

To analyse the spectroscopy background, the assignment of spectral bands to specific vibrational transitions of molecular functional groups was then performed based on regression coefficients from PLS-DA for each of the classes using spectral atlas ¹¹. The further from zero the regression coefficient was, the more influence on classification the given spectral band has. The most influential bands for classification are shown in Figure 25.

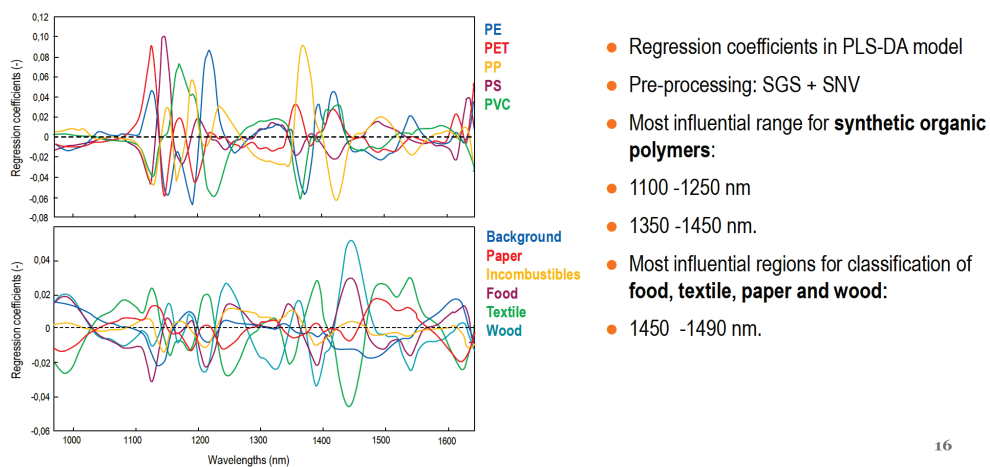


Figure 25: Most influential bands for classification

¹¹ Workman J. and Weyer L. (2012) *Practical Guide and Spectral Atlas for Interpretive Near-Infrared Spectroscopy*. CRC Press, Boca Raton. 326 pages. ISBN 1439875251.

Overall, it can be concluded that HSI is a good candidate to determine the moisture content and ash content in biomass samples. HS imaging can present individual pixel value estimations of moisture and ash content in the same sample i.e., it provides both spatial and spectral information. This can be interesting when measuring and monitoring moisture, ash content etc. in biomass feedstock for industrial purposes.

The results demonstrated that it is possible to develop a classification model that can recognize most common components of RDF based on NIR-HSI data. The models developed based on machine learning methods can successfully classify pixels belonging to textile, wood, food, paper, and most common types of plastics with reasonable accuracy. Nevertheless, classification of materials with no specific absorbance spectrum in the NIR region such as metals, glass, or ceramics is more challenging.

From a model accuracy perspective, it can be seen that traditional PLSR model give the best result for woody biomass. Nonetheless the ANN model is also very promising particularly if the number of samples which in this was very small could be increased. Hence, ANN could be a promising technique for HSI as it can deal with large datasets and the accuracy will get better as the number of samples increases.

For RDF classification traditional PLS-DA achieved the worst accuracy levels. In comparison RBNN and SVM both achieved higher accuracy but at the cost of one and two orders of magnitude higher computation time, respectively. For real-time applications with relatively low available computational power (embedded system) this may pose a significant short-term limitation but will most likely be less significant in the medium term and processor technology evolves.

It is noted that NIRS-based HSI employing deep-learning approaches for estimating particle size distribution in biomass processes has very good potential; it also poses significant challenges in signal acquisition and treatment. It is nonetheless a pioneering approach, never implemented before in the biomass-based CHP field, and the learning curve with HSI within the OptiC-NIRS project has been steep.

RAMAN SPECTROSCOPY

Apart from using traditional FT-NIR and DA-NIR measurement systems, as well as an HSI NIRS camera, Raman spectroscopy was also investigated within OptiC-NIRS. Raman is a spectroscopic technique used to observe vibrational, rotational, and other low-frequency modes in a system. The technique is based on the light scattering of molecules using a monochromatic light source (laser) and effectively provides a fingerprint by which molecules can be identified.

Raman scattering occurs when a photon transfers its energy resulting in a change in the wavelength of the photon and hence inelastic diffusion (Raman). There are two different types of Raman diffusion, the Stokes and the anti-Stokes diffusion, depending on whether the photon loses or gains energy, respectively. Raman is

complementary to Mid-IR with different intensities and selectivity. Key aspects to note is that it is based on polarizability (instead of polarity), no need of sample preparation, water doesn't interfere on Raman spectra, diatomic molecules like gas can be detected.

The unit utilised within OptiC-NIRS was a HORIBA Raman spectrophotometer with two different lasers, 735nm and 1064nm, and optic fiber heads. This is an experimental customised system and is shown in Figure 26, along with a schematic of the basic measuring principle of the Raman technique.

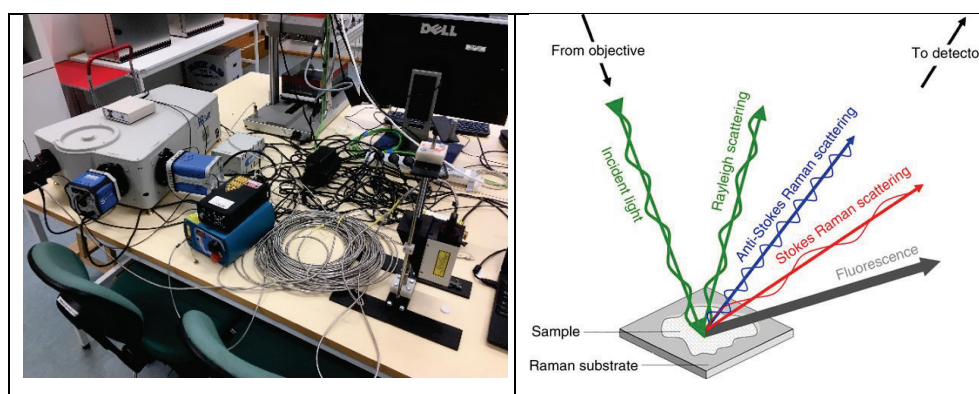


Figure 26: Experimental Raman system employed within the project and measuring principle

It is noted that the intensity of Raman scattering is greatly increased by using shorter-wavelength lasers. Nonetheless, the Raman effect is an extremely weak phenomena, with very low conversion efficiencies. Therefore, the signal can easily be overwhelmed by autofluorescence from the analyte. Unfortunately, organic and biological materials tend to have broad autofluorescence in the visible spectrum and hence longer-wavelength lasers are preferable. In the case of 1064nm excitation, the signal is nonetheless very weak, and the detector (InGaAs) will have a noisy resolution (in wavenumbers) is very poor, despite Raman scattering efficiency being fairly high in the deep-UV region. Using 785nm excitation is in some cases preferred as it is the longest-wavelength laser source that still allows for fairly wide spectra range using silicon detectors, but fluorescence can be a significant problem.

During sample testing it was noted that the inner part of the wood gives a better signal, with relatively lower fluorescence, with a minimum exposure time of 1min. Bark on the other hand absorbs all the laser energy and can combust very fast (in principle after 1s of exposition to the laser). Longer exposure times may be needed for different samples, as shown in Figure 27, but this needs to be balanced against potential fire hazards. For a detailed presentation of the intricacies of analysing woody biomass using Raman spectroscopy the interested reader is referred to the excellent work presented in ¹².

¹² Anni Lähdetie. (2013) *Wood Biomass Characterization by Raman Spectroscopy*. PhD thesis, Aalto University. Finland. (<http://urn.fi/URN:ISBN:978-952-60-5469-8>)

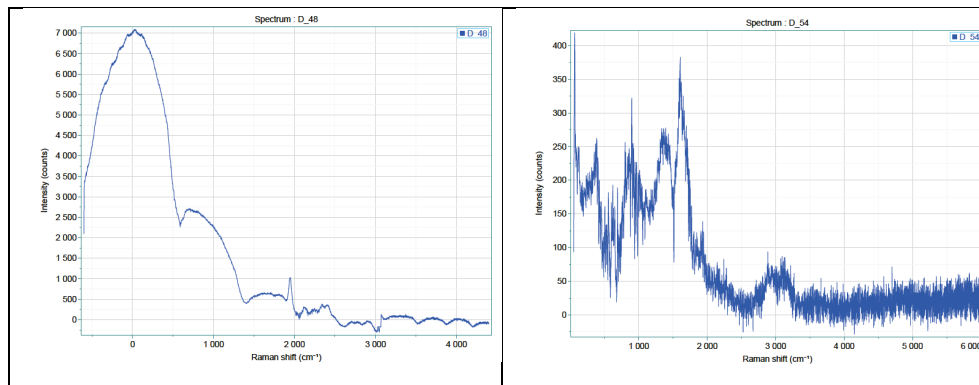


Figure 27: Example of difference in spectra samples from varying exposure time

Some of the cellulose/lignin peaks are in principle visible on the spectra, and some data treatment (Pearson's baseline correction) may give a good enough signal for peak interpretation, as illustrated in Figure 28 and Figure 29.

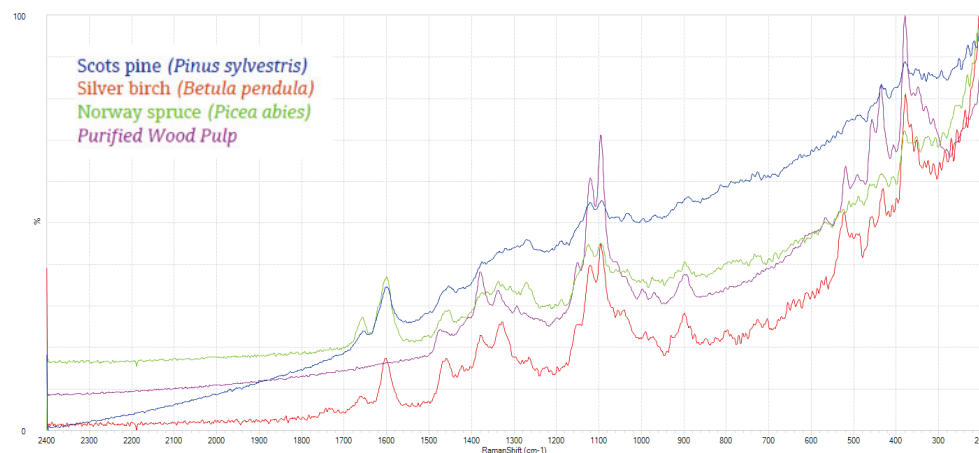


Figure 28: Example spectra of cellulose/lignin peaks for different materials (no pre-processing)

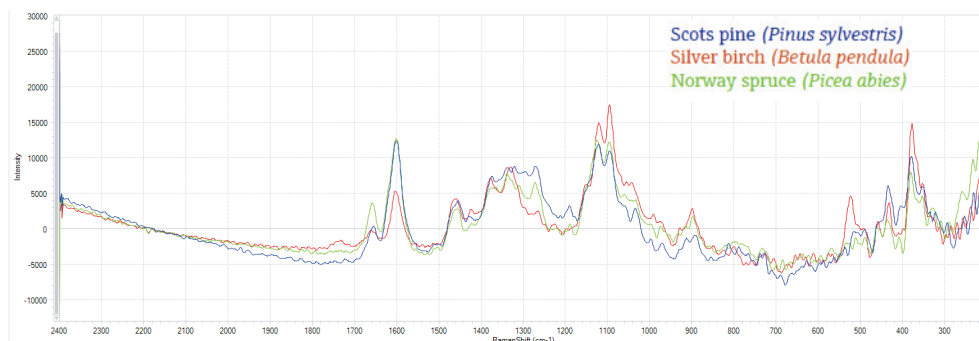


Figure 29: Example spectra of cellulose/lignin peaks for different materials (Pearson's baseline correction)

Overall, the spectra acquired were found to be exploitable for distinguishing between different tree species, but inappropriate for the purposes of building a

robust soft-sensor for measuring fuel material properties such as higher heating value and ash content. Moreover, the long exposure times make an on-line application impractical, while the issue with sample combustion creates a significant hazard for a practical installation of a Raman instrument over a conveyor belt. Based on these findings it was decided to not proceed with a full-scale demonstration of the Raman sensor, and instead focus on traditional NIR and HSI.

3 Full-scale Demonstrations

Following the lab-scale work presented in the previous section, NIRS soft-sensors were consequently in full-scale industrial demonstration at the facilities of Eskilstuna Strängnäs Energi och Miljö AB (ESEM) and Mälarenergi AB. Experiences from these demonstrators are presented in the sub-sections below.

INSTALLATION AT ESEM

Several NIRS instruments were installed at the facilities of ESEM, in Eskilstuna, Sweden, for the available combustion system, namely a bubbling fluidized-bed boiler, that burned biomass-derived fuel i.e., woodchips. The demonstration included the design, construction and installation of an appropriate instrument holder. The demonstration process had to undergo several tests and iterations due to safety concerns, hazards and the overall complexity of the industrial environment where the sensors were installed. Selecting an optimal sensor location is challenging, and rarely can the requirement be achieved to measure the fuel right before it ends up in the boiler, limited in principle by constraints in the facility design.

For comparative purposes, two different instruments based on two different measuring principles, were installed. They were both so-called traditional NIR instruments, with the first instrument (Bruker) relying on Fourier Transformation technique using a robust interferometer to acquire very strong signals. The second instrument (Buchi) was based on the Diode Array technique being able to acquire signal for all the spectral intervals at the same time.

It proved possible to maintain an approximately constant sample-to-sensor distance, in order to ensure focus of the sensor and hence high quality NIR spectra capturing. This was successfully achieved through the design and construction of an appropriate instrument holder. This was far from a trivial task and required a considerable amount of time to be invested in the design of the instrument holder as shown in Figure 30, as well as Figure 31 and Figure 32.



Figure 30: Instrument holder as installed on-site

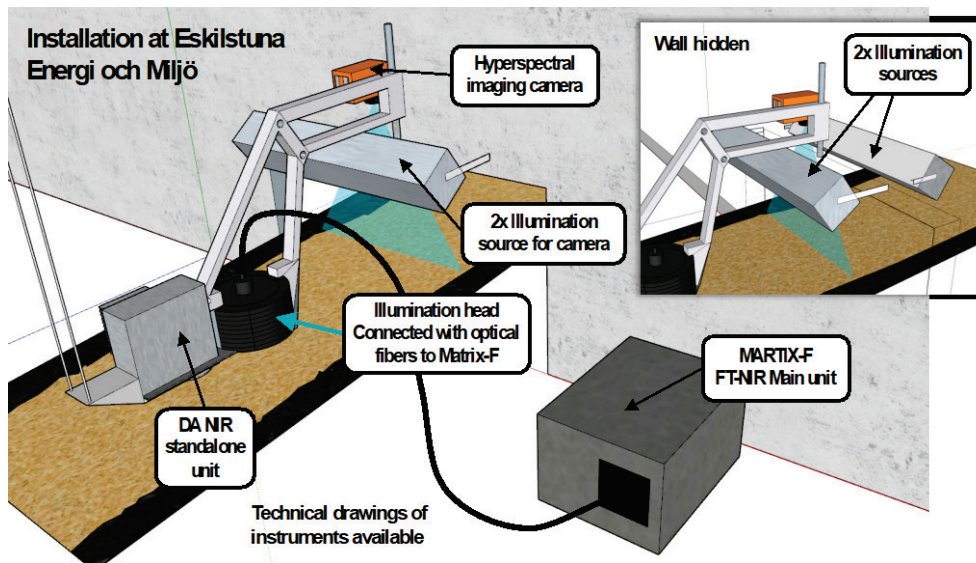


Figure 31: Installation of NIRS instruments at ESEM (view 1)

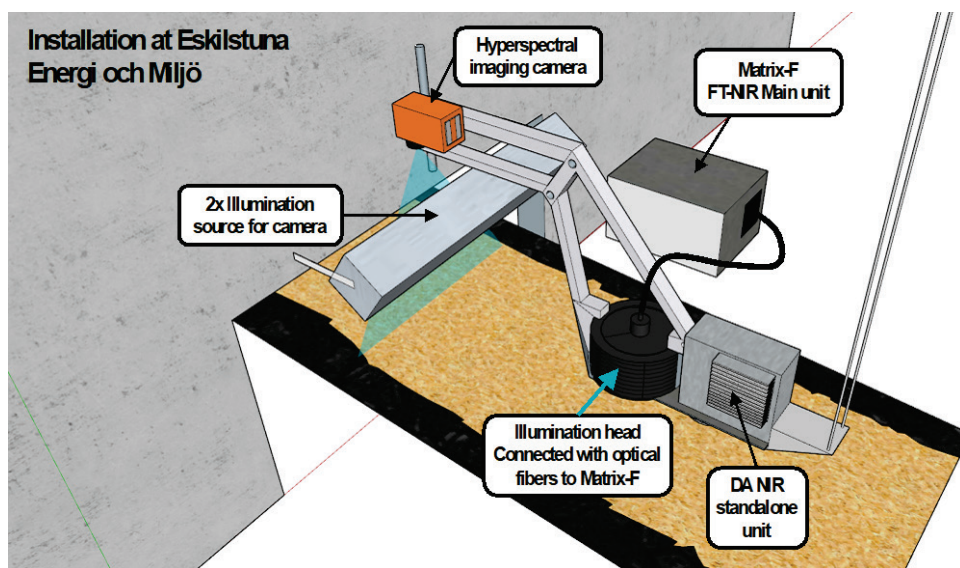


Figure 32: Installation of NIRS instruments at ESEM (view 2)

Among other requirements, the instrument holder must ensure:

1. The sensor-head will never fall into the conveyor belt (and hence end up in the boiler).
2. Variations in fuel level in the belt do not significantly affect the distance between fuel and sensor-head.
3. The sensor-head can be unmounted while the conveyor belt is still running at full speed and fuel level.
4. Dust is not built up around hot parts of the instruments, and hence no fire hazard can be caused by the installation.

- All equipment mounted on the holder over and around the conveyor belt follows the ATEX classifications set for the specific environment as part of the facility insurance.

Apart from installing the sensors, it is important to have a practical solution for piping the acquired signal to the decision support system used by the operator. A schematic of how the connections of the instrumentation to the powerplant infrastructure were carried out for the purposes of the demonstration is given in Figure 33. The focus is on transferring the signals from the location they are taken (conveyor belt) to the location they are needed (control room). In a commercial installation it is expected that any intermediate connections within the soft-sensor system is avoided (at best be part of a certified embedded system) with focus on direct connections to the local DCS/SCADA system, and Historian (database), using standard TCP/UDP and ModBus communication protocols.

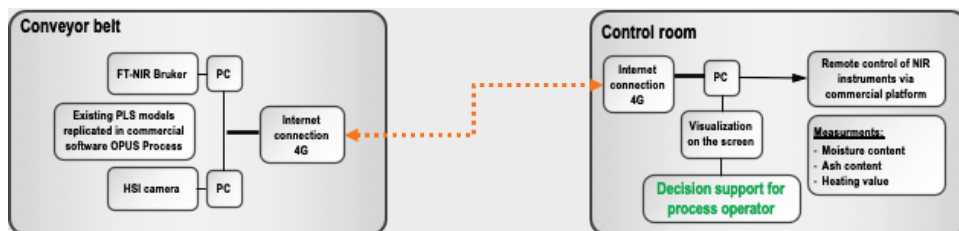


Figure 33: Connection of instrumentation to powerplant control room

As discussed in the previous section, labs-scale calibrations based on the hyperspectral imaging technique were also developed. As a result, the installation of a hyperspectral imaging camera was also carried out as part of the demonstration activity under the OptiC-NIRS project.

Practical HSI camera implementations require a strong lighting system, with appropriate industrial-grade installation for the lighting system ensuring no fire hazard from glass overheating and dust depositions. In the case of the present HSI camera installation, the lighting source was incorporated in the demonstrator, as shown in Figure 34. Key design considerations included appropriate industrial-grade installation for the lighting system ensuring no fire hazard from glass overheating and dust depositions.

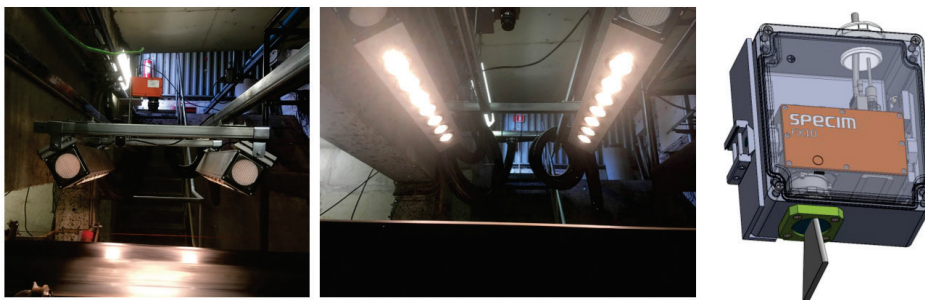


Figure 34: Lighting arrangement for HSI system

Further practical challenges to address included setting optimal distance in the presence of fluctuations in the feedstock level as well as dealing with vibrations. Finally, it is imperative that the camera system is able to take pictures at a very high framerate if the conveyor belt is moving very fast. The expectation would be for a capability of at least 500 frames per second for conveyor belt speeds in the range of 1-2m/s. Underlying algorithms for real-time post-processing of such large amounts of data, and appropriate solutions for storing only the data needed are also required.

Continuous signals were acquired from all the installed NIR sensors over a period of time. A practical solution was established so that the data can be transferred in real-time to the operation station from where the boiler operation was monitored and effectively adjusted. Examples of the actual soft-sensor estimations (signals) for key biomass fuel properties as they came during the demonstration are given in Figure 35. These estimations came from the calibrations of the installed sensors based on the spectra of the actual feedstock as acquired online over the conveyor belt. The signal frequency was approximately 20s and the plots are showing fuel feed variations for a period of approximately 45 minutes.

It must be noted here that the moisture content (solid black line) is not correlated to the higher heating value (dashed grey line). The reason is that this higher heating value estimate is on dry basis and hence excludes the effects of wood-chip moisture i.e., the value given by the soft-sensor is the one that would correspond to the bomb calorimeter value if the wood chips had been dried before applying the reference method. For the case of MPC demonstration, the higher heating value signal is of course further corrected using the measured moisture content signal and the correlations available in the open literature for going from dry basis to an effective heating value for moist wood chips.

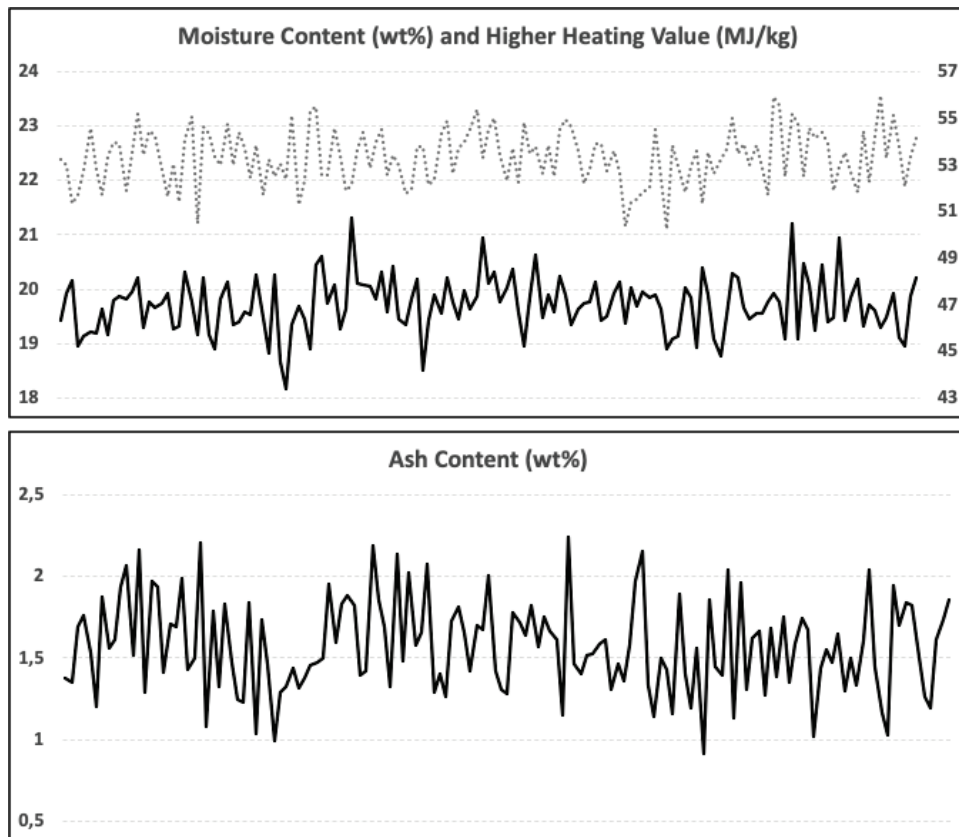


Figure 35: Examples of the actual soft-sensor estimations (signals) for key biomass fuel properties

INSTALLATION AT MÄLARENERGI

A further full-scale demonstration has been carried out at the facilities of Mälarenergi AB in Västerås, Sweden. The aim here was to test the NIRS sensors on a different type of combustion system, a circulating fluidized bed boiler, with a different type of fuel, namely refuse-derived fuel (RDF). This was a particularly challenging installation as finding an appropriate location for installing the NIRS sensors had to go through a set of very stringent environmental safety constraints.

Figure 36 shows the location of the sensor installation where it becomes clear that this was on a fully closed conveyor belt, with very limited access, resulting in a rather complicated installation. More details of the NIRS head installation are shown through Figure 37, while a boroscope view of the NIRS head measuring over the conveyor belt is given in Figure 38.

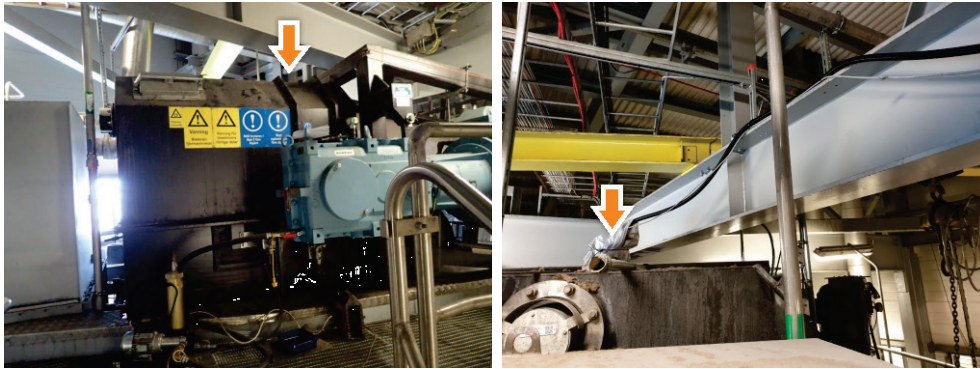


Figure 36: Installation location at Mälarenergi



Figure 37: Details of NIRS head installation over the conveyor belt at Mälarenergi

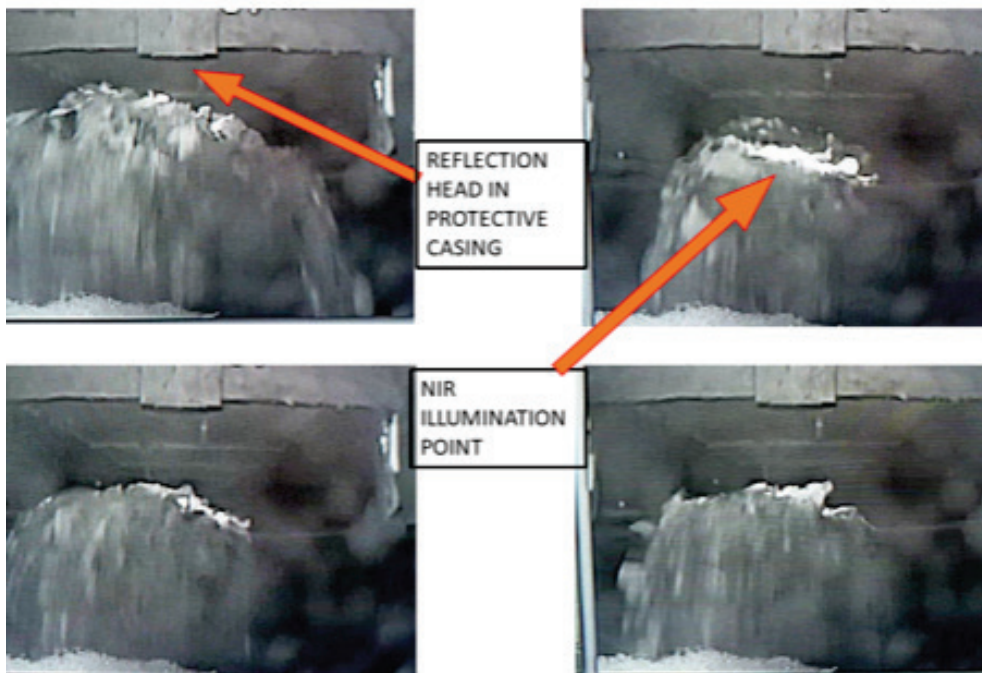


Figure 38: Boroscope view of NIRS head measuring over the conveyor belt at Mälarenergi

The acquired data in this case, and based on the experiences from the ESEM demonstration, were transferred directly to the dedicated Historian (database) system of Mälarenergi. A number of predicted parameters like RDF moisture content, heating value and combustible fraction, are made available directly on the DCS / SCADA system ABB 800XA, as well as the ERP-level monitoring platform ABB Ability. The detailed arrangement is illustrated in Figure 39.

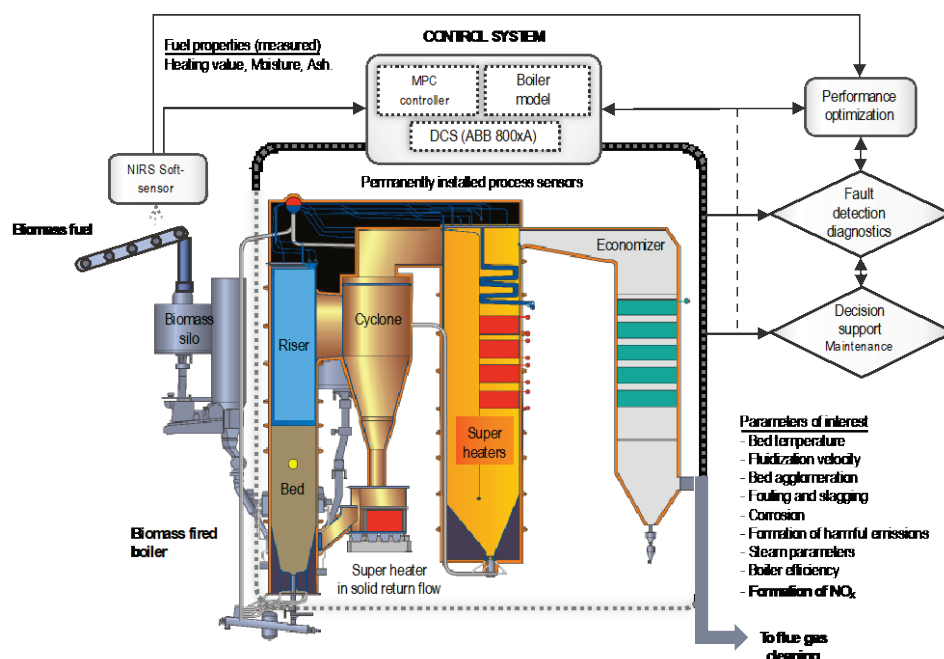


Figure 39: Circulating fluidized bed boiler at Mälarenergi

A qualitative comparison was made between the NIRS-based moisture predictions and the water content measurements performed in the flue gas downstream of the boiler. There was an approximate 45 minutes delay between the NIR measurement and the flue gas analysis, and the data have been corrected/synchronized accordingly. The white noise in the measurements was filtered using a 15-minute moving average, which works reasonably well. The results in Figure 40 show that the two measurements were well correlated, considering the variation in the process and fuel feedstock, and the white noise in the measurements themselves.

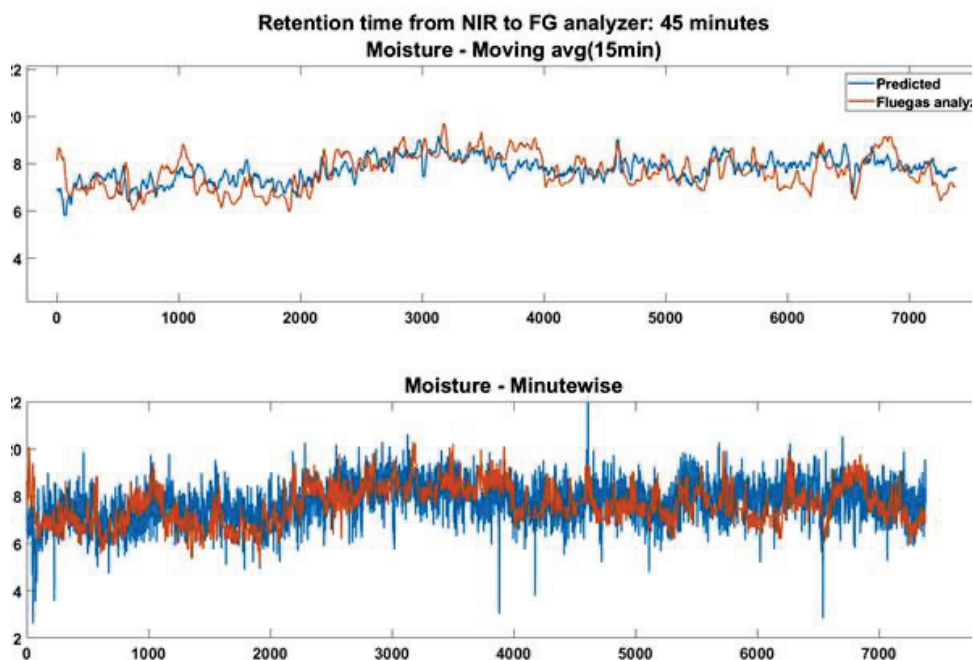


Figure 40: Comparison of NIRS moisture predictions and flue gas analysis with 45-min delay applied: (top) 15-min moving average signals; (bottom) 1-min signals

Within the ABB Ability platform, a physics-based dynamic model has been incorporated and coupled to a feed-forward model predictive control (FFMPC) simulator. The system is using the NIR soft-sensor predictions to provide suggestions for improved real-time control of the RDF-fired boiler system. The developed FFMPC simulator system that has been implemented on-line at Mälarenergi for providing operator decision support is illustrated through Figure 41. It can be noted that although the FFMPC received the on-line signals from the powerplant, the effect of the actuator movements on the boiler performance was simulated using the physics-based model. The resulting outcome was displayed into the control room as relevant decision support information for the powerplant operators. In a future demonstration, the ambition would be to allow the MPC to take over the actuator movement vs the current industrial control approach implemented.

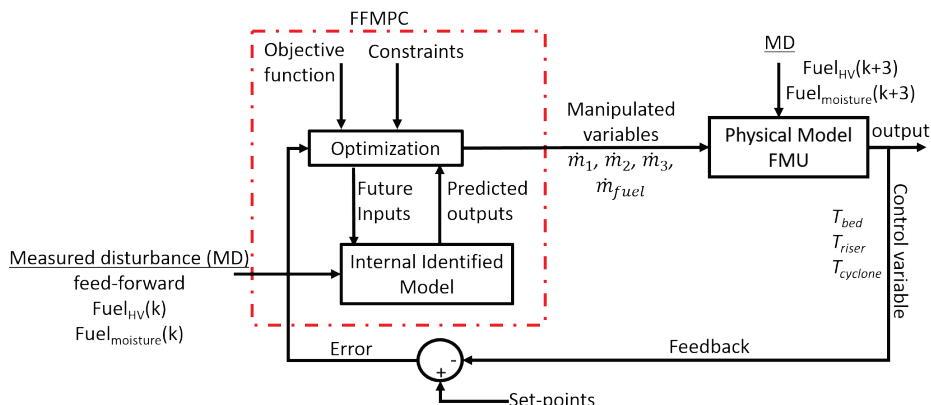


Figure 41: The feed-forward model predictive control on-line simulator implemented at Mälarenergi

Different actuators (the manipulated variables) are manipulated by the proposed FF MPC approach, to compensate for measured disturbances in the RDF feedstock fuel heating value and moisture content, as measured using the NIRS soft-sensors. Key parameters that are being manipulated include fuel feeding rate, primary air flow rate, secondary air flow rate and tertiary air flow rate. These are illustrated in Figure 42.

The quality of the achieved set point stability is illustrated in Figure 43. Through this on-line simulator analysis using as input the NIRS-soft sensor signal (the measured disturbances), it is shown that boiler and cyclone temperatures can be controlled to an accuracy at least as good as what can be measured using practical measurement techniques. The achievement of approximately 1K accuracy is an order of magnitude improvement vs current industrial control.

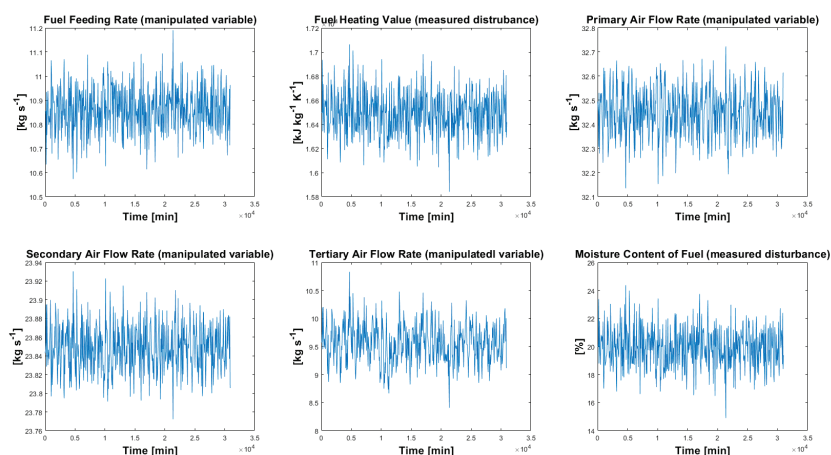


Figure 42: Actual measured disturbances and FF MPC manipulated variable (actuator) suggestions

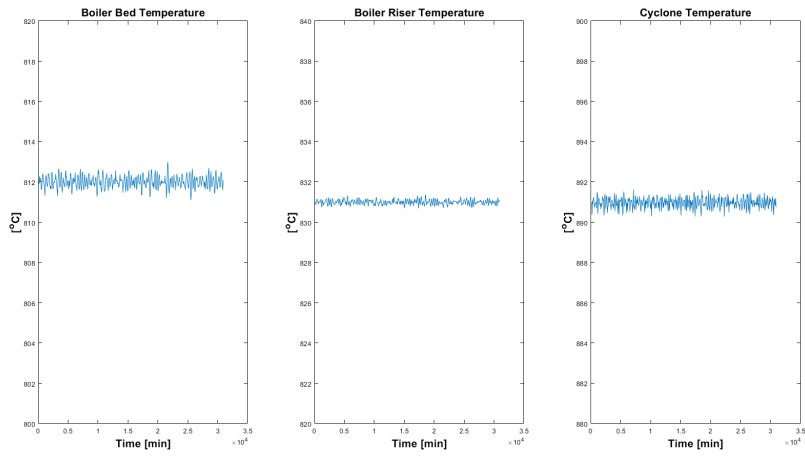


Figure 43: FFMPC control variable simulator results

4 Conclusion and Lessons Learnt

The overall aim of the project was to evaluate the potential of using NIR measurements as soft sensors for the on-line characterisation of biomass and RDF material properties. A combination of lab-scale experiments and full-scale demonstrations were successfully carried out.

LAB-SCALE EXPERIMENTS

It was possible to develop lab-scale traditional NIRS calibration models with accuracy well within a couple of % units (after model optimization process) for both moisture content and higher heating value. Ash content was more challenging but accuracies within 0.5% were shown to be possible. It can also be concluded that the employment of less traditional machine learning techniques (such as GPR, instead of PLS) has led to significant improvements in model accuracy. Nonetheless, NIRS prediction models will need to be improved continuously through the re-training/validating the algorithm by adding new reference/spectral data, particularly when the model is running on-line with real time data.

Hyperspectral NIR imaging was found to be a very good candidate to determine the moisture content and ash content in biomass samples, with accuracy levels similar to that of traditional NIRS. HS imaging can present individual pixel value estimations of moisture and ash content in the same sample i.e., it provides both spatial and spectral information. This can be interesting when measuring and monitoring moisture, ash content etc. in biomass feedstock for industrial purposes.

The results demonstrated that it is possible to develop a classification model that can recognize most common components of RDF based on NIR-HSI data. The models developed based on machine learning methods can successfully classify pixels belonging to textile, wood, food, paper, and most common types of plastics with reasonable accuracy. Nevertheless, classification of materials with no specific absorbance spectrum in the NIR region such as metals, glass, or ceramics is more challenging.

From a model accuracy perspective, it can be seen that traditional PLSR model gives the best result for woody biomass. Nonetheless the ANN model is also very promising particularly if the number of samples - which in this work was very small - could be increased. Hence, ANN could be a promising technique for HSI as it can deal with large datasets and the accuracy will get better as the number of samples increases.

For RDF classification traditional PLS-DA achieved the worst accuracy levels. In comparison RBNN and SVM both achieved higher accuracy but at the cost of higher computational time. For real-time applications with relatively low available computational power (old embedded systems) this may pose a limitation. Still, this will most likely be less significant in the medium and longer term, since modern embedded systems have increasingly higher computational power enabling

predictions from all the aforementioned methods that are faster than the instrument sampling time.

It is noted that NIRS-based HSI employing deep-learning approaches for estimating particle size distribution in biomass processes has very good potential; it also poses significant challenges in signal acquisition and treatment. It is nonetheless a pioneering approach, never implemented before in the biomass-based CHP field, and the learning curve with HSI can be steep.

Raman spectroscopy was also explored within the OptiC-NIRS project. Overall, the spectra acquired were found to be exploitable for distinguishing between different tree species, but inappropriate for the purposes of building a robust soft-sensor for measuring fuel material properties such as higher heating value and ash content. Moreover, the long exposure times make an on-line application impractical, while the issue with sample combustion creates a significant hazard for a practical installation of a Raman instrument over a conveyor belt. Based on these findings it was decided to not proceed with a full-scale demonstration of the Raman sensor, and instead focus on traditional NIR and HSI.

FULL-SCALE DEMONSTRATIONS

The accuracy of the on-line NIRS system is naturally expected to be lower than what was demonstrated in the controlled conditions of the SPECTRA lab environment. In the full-scale implementation, the speed and fuel level in the conveyor belt will vary significantly and continuously. The temperatures at which the NIRS sensor have to take measurements vary during the day as well as with the seasons, with significant low temperature extremes during winter; the humidity of the ambient air also varies and can affect measurements during certain days. Furthermore, the exact accuracy of the soft-sensor is not possible to verify on the conveyor belt since the samples scanned are led directly to the boiler and cannot be isolated for further chemical analysis using reference methods. But even if that was possible, the variations in fuel material properties over a period of few weeks during winter are considerably smaller than what has been investigated during the lab-scale work. Nonetheless, the NIRS system is considered to be sufficiently accurate, particularly if calibrated on-site, and can provide reliable “delta” information for use by the control system for optimal operation of the boiler with varying feed-stock quality.

During the demonstrations, it proved possible to maintain an approximately constant sample-to-sensor distance, in order to ensure focus of the sensor and hence high quality NIR spectra capturing. This was successfully achieved through the design and construction of an appropriate instrument holder. This was far from a trivial task and required a considerable amount of time to be invested in the design of the instrument holder.

In a commercial installation it is expected that any intermediate connections within the soft-sensor system is avoided (at best be part of a certified embedded system) with focus on direct connections to the local DCS/SCADA system, and Historian (database), using standard TCP/UDP and ModBus communication protocols.

Practical HSI camera implementations require a strong lighting system, with appropriate industrial-grade installation for the lighting system ensuring no fire hazard from glass overheating and dust depositions. Further practical challenges to address include setting optimal distance in the presence of fluctuations in the feedstock level as well as dealing with vibrations. Finally, it is imperative that the camera system is able to take pictures at a very high framerate if the conveyor belt is moving very fast. The expectation would be for a capability of at least 500 frames per second for conveyor belt speeds in the range of 1-2m/s. A resolution of 640 pixels will most likely suffice for practical on-line applications for biomass and RDF. Underlying algorithms for real-time post-processing of such large amounts of data, and appropriate solutions for storing only the data needed are also required.

OUTLOOK AND FUTURE WORK

Through these demonstrations, it was shown that it is possible to implement model-predictive feed-forward control on modern biomass and RDF-fired fluidised bed boilers. Boiler and cyclone temperatures could be controlled to an accuracy at least as good as what can be measured using practical measurement techniques. The key enabling technology - for the feed-forward signal of the feedstock material properties - are the NIRS soft-sensors. It is the recommendation of the authors of this report that the technology is brought forward to commercial level, and NIRS soft-sensors find wide use in on-line characterisation of biomass and RDF in combined heat and power plants, in Sweden as well as other parts of the world.

It is hoped that OptiC-NIRS project has helped progress the technology readiness level of NIRS system for on-line measurements of biomass and RDF. This by reducing risks in full-scale implementations and by providing useful lessons learnt for taking the technology to the next level. A commercial implementation of these concepts would be the natural step in a future (commercially oriented) full-scale technology demonstration project. It is considered that the work remaining for bringing the shortlisted investigated technologies as a new product in the market, is in principle non-academic, and to some extent will be specific to the chosen installation site, the commercial sensor head/detector, and the particularities of the fuel in use. The list of lessons learnt provided in this report should go a long way in reducing the time and effort needed to materialise each new installation/implementation.

Finally, it is noted that the following aspects have not been investigated within the OptiC-NIRS project, but could be points for investigation within future (academic-oriented) projects:

1. Correlations between the humidity measured in the flue gas and the woody biomass humidity as measured by NIRS soft-sensors, corrected for the use of water spraying downstream of the sensor.
2. Development and consistent utilization of methods for establishing the accuracy of the developed soft-sensors on-site as installed over the conveyor belt.
3. Identification of the fossil part of refuse-derived fuel.
4. Utilisation of Laser-Induced Breakdown Spectroscopy for refuse-derived waste fuel analysis with particular focus on inorganic (sub-) components of the latter.

Appendix A: Aim and Objectives

The overall aim of the project was to evaluate the potential to use NIR measurements as soft sensors for the on-line characterisation of biomass and waste material properties for diagnostics and optimal control of combined heat and power plants.

The specific objectives set were:

1. Transfer existing laboratory NIR calibrations for biomass and waste material properties to a combined heat and power plant's online biomass handling system.
2. Use the soft sensor signals as input to powerplant control and evaluate the possibility for process control i.e.,
 - a. What on-line accuracy can be achieved?
 - b. How does the optical sensor type and distance from the feedstock, as well as conveyor belt speed, influence the quality of the SPECTRA measurements and resulting determination of fuel heating value, moisture, components such as recycle wood and glass, different type of plastics and ash?
3. Implement the system on-line along with other available sensors and dynamic models at the Mälarenergi and Eskilstuna Strängnäs Energi och Miljö powerplants. Use the integrated system for determining key parameters such as fuel feed volume and providing useful input for control to the line operators.
4. Evaluate the benefits from the on-line implementations at the Mälarenergi and Eskilstuna Strängnäs Energi och Miljö powerplants. The evaluation of the implementation test results will be carried out together with the powerplant staff.

ACHIEVEMENT OF PROJECT OBJECTIVES

With regard to the first objective, the project focused on two different installation locations i.e., Mälarenergi in Västerås and Eskilstuna Energi och Miljö in Eskilstuna. The demonstrations were carried out successfully in both locations.

With regard to the second objective, the accuracy achieved is deemed sufficient for online-process control, particularly when considering feed-forward model-predictive control. The current industrial control practice makes no consideration for such input signals so this a step development in practical CHP control.

For FT-NIR the optimal distance was found to be in the order of 14cm, but it is difficult to maintain this distance in a practical installation due to safety considerations since the feedstock level can vary considerably. As a result, a higher distance has to be chosen but the trade-off is acceptable.

The conveyor belt speed can affect the quality of the prediction and it is therefore that reference spectra samples taken in the lab are not static. Nonetheless this is not

a showstopper and good calibrations can be developed. For HSI cameras it is imperative that the system is able to take picture at a sufficiently high frame rate. Vibrations however merit special consideration for HSI systems, albeit mature FT-NIR system with robust interferometers do not suffer considerably by such challenges.

With regard to the third objective, and similar to the soft-sensor demonstration, the control techniques have also been demonstrated successfully. A particular challenge in this case related to storing the information produced in real time in the local database system and making it available for use in the actual DCS, SCADA and ERP-level systems. The most complex case was that of Mälarenergi as it involved linking together several industrial systems (ABB 800XZ, ABB Ability, Dockers and FMI, Tieto HMI3) some of which contained classified data and required special permissions and check by SÄPO.

With regard to the fourth objective, the overall capability developed is superior to current industrial control practices. By knowing the quality of the incoming feedstock, it was found that a much tighter control of different system parameters can be achieved, for example boiler temperature. At the same time much smaller actuator movements are needed which can help the equipment to last longer and reduced maintenance costs. The underlying systems can enable to move on the next stage of online and remote diagnostics as well as predictive maintenance.

DEVIATIONS FROM PROJECT OBJECTIVES

The use of Raman spectrometer albeit promising at lab level has proven to have too many challenges that need to be overcome in order to reach a practical implementation/demonstration stage. It has been established in the project that a large amount of time is needed in order to acquire spectra of appropriate quality which is challenging with current conveyor belt speeds. Also, the sensitivity of the sample to sensor distance (when away from optimal conditions) results in extremely weak signals for feedstock with even small level variation. Finally, the high risk of ignition of biomass and RDF feedstocks required very detailed safety assessments; in fact, the high energy laser that gives the best result has also the highest risk of ignition. Therefore, this project concludes that it is NIR hyperspectral imaging (NIR-HSI) technology that is the most promising next step from traditional FT-NIR and DA-NIR, rather than Raman spectroscopy.

Appendix B: Publications

The key publications stemming out of the OptiC-NIRS project are listed below:

1. Mobyen Uddin Ahmed, Peter Andersson, Tim Andersson, Elena Tomas Aparicio, Hampus Baaz, Shaibal Barua, Albert Bergström, Daniel Bengtsson, Daniele Orisio, Jan Skvaril, Jesús Zambrano. *A Machine Learning Approach for Biomass Characterization*. Energy Procedia, 158, 1279-1287. Presented at 10th International Conference on Applied Energy. 2018.
2. Nathan Zimmerman, Konstantinos Kyprianidis, Carl-Fredrik Lindberg. *Waste Fuel Combustion: Dynamic Modeling and Control*. Processes, 6(12):222, 2018.
3. Martin Sevçik. *Near-Infrared Spectroscopy for Refuse Derived Fuel Characterization: Classification of waste material components using hyperspectral imaging and feasibility study of inorganic chlorine content quantification*. Mälardalen University, MSc thesis, Västerås, Sweden, 2019.
4. Jerol Soibam, Ioanna Aslanidou, Mikael Karlsson, Konstantinos Kyprianidis. *Hyperspectral Imaging of Biomass Fuels for Moisture Content Using Machine Learning Techniques*. Presented at the 19th International Conference on Near Infrared Spectroscopy - NIR 2019, Gold Coast, Australia, 15-20 September 2019.
5. Jan Skvaril, Seyedpedram Khalesimoghdam, Jerol Soibam, Konstantinos G Kyprianidis, Monica Odlare. *Application of single-point and hyperspectral imaging near-infrared sensors and machine learning algorithms for real-time biomass characterization Techniques*. Presented at the 19th International Conference on Near Infrared Spectroscopy - NIR 2019, Gold Coast, Australia, 15-20 September 2019.
6. Martin Sevçik, Jan Skvaril, Elena Tomas Aparicio. *Applications of hyperspectral imaging and machine learning methods for real time classification of waste stream components*. Presented at the 19th International Conference on Near Infrared Spectroscopy - NIR 2019, Gold Coast, Australia, 15-20 September 2019.
7. Milan Zlatkovikj, Valentina Zaccaria, Ioanna Aslanidou, Konstantinos Kyprianidis. *Simulation Study for Comparison of Control Structures for BFB Biomass Boiler*. Proceedings of the 61st International Conference of Scandinavian Simulation Society, SIMS 2020, Paper ID 27, Linköping University Electronic Pres. September 2020.

ON-LINE POWERPLANT CONTROL USING NEAR-INFRARED SPECTROSCOPY

Att känna till så mycket som möjligt om det biobränsle man använder är viktigt för energibranschen. Här har forskarna utvärderat möjligheten att använda mätningar av nära infrarött, NIR för att kunna bestämma olika egenskaper hos biomassa.

Genom att i realtid få information om fukthalten på bränslet kan man få en mer stabil förbränningstemperatur, en effektivare förbränning som ger reducerade utsläpp av kväveoxid och en bättre bränsleekonomi.

Resultaten visar att man med hjälp av OptiC-NIRS kan styra och kontrollera förbränningsprocesserna inom kraft- och värmebranschen. Det är ett antal olika egenskaper i bränslet som är av intresse för processen, framför allt halten fukt. Andra egenskaper som också är bra att känna till är värmevärde, askhalt, innehåll av glas och av fossilt material exempelvis plaster.

Energiforsk is the Swedish Energy Research Centre – an industrially owned body dedicated to meeting the common energy challenges faced by industries, authorities and society. Our vision is to be hub of Swedish energy research and our mission is to make the world of energy smarter!