PSO 4881
Modelling of bio-power stations
Development of co-firing

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Doc. no. 929952
(ver. no. 929952A)

Project initiated: **1 January 2004**
Project terminated: **31 December 2011**
Project objective: **To develop a modelling tool verified through laboratory tests and pilot as well as full scale plant tests to predict the consequences of co-firing at future power stations.**

1.   Background

The primary challenges in terms of boiler operation in connection with co-firing of biomass at central power stations are corrosion, catalyst deactivation, burn-out conditions, emissions (primarily NOx) and reuse of fly-ash.

Based on the intention to increase the share of biomass used for power production in Denmark this project was established to improve the basic understanding of co-firing of straw including the modelling tools used for analysis of the consequences for future plant conversions. The project did not include investigation of catalyst deactivation, which has been treated in previous projects, and did not engage in fly-ash utilization.

DONG has developed co-firing of biomass at the company's coal fired stations through a no. of years. The present project is a direct continuation of a number of earlier projects such as PSO 4105: Biomass co-firing in Suspension-Fired Power Plants, which were reported 2008.

The project was divided into the following sub-projects and activities:
1. *PSO 4766: Ash transformation*. Investigation of the interaction between fuel composition and the composition of fly ash and deposits with emphasis on potassium, chlorine and sulphur.
2. *PSO 4788: Corrosion collaboration*. Continuation of the work to understand the interaction between the composition of flue gas and deposits from co-firing and the derived corrosion mechanisms for steel types applied.
3. *PSO 4805: Channel formation.* Quantification of possible consequences of localised high biofuel shares in power plant boilers in connection with co-firing where the co-fired fuel is fed into few burners.
4. *PSO 4806: Low-NOx burner*. Development of an improved modelling tool for prediction of NOx emissions when changing burners to co-firing/multi-fuel firing.

2.   Key results

2.1   PSO 4788: Corrosion collaboration

Superheater and reheater test sections exposed to co-firing of biomass and fossil fuels for up to four years were investigated. The samples originated from the Studstrup unit 4 boiler co-firing coal and straw (at 10% thermal biomass share) and the Avedøre unit 2 boiler co-firing wood pellets with heavy oil and gas at various biomass shares (from 0-100%).

Corrosion rates obtained for 1, 2, 3 and 4 years of exposure were compared with rates established during the co-firing demonstration campaign at Studstrup unit 1 involving straw shares of 0-20% (thermal) and 3000 hours of exposure (Figure 1).
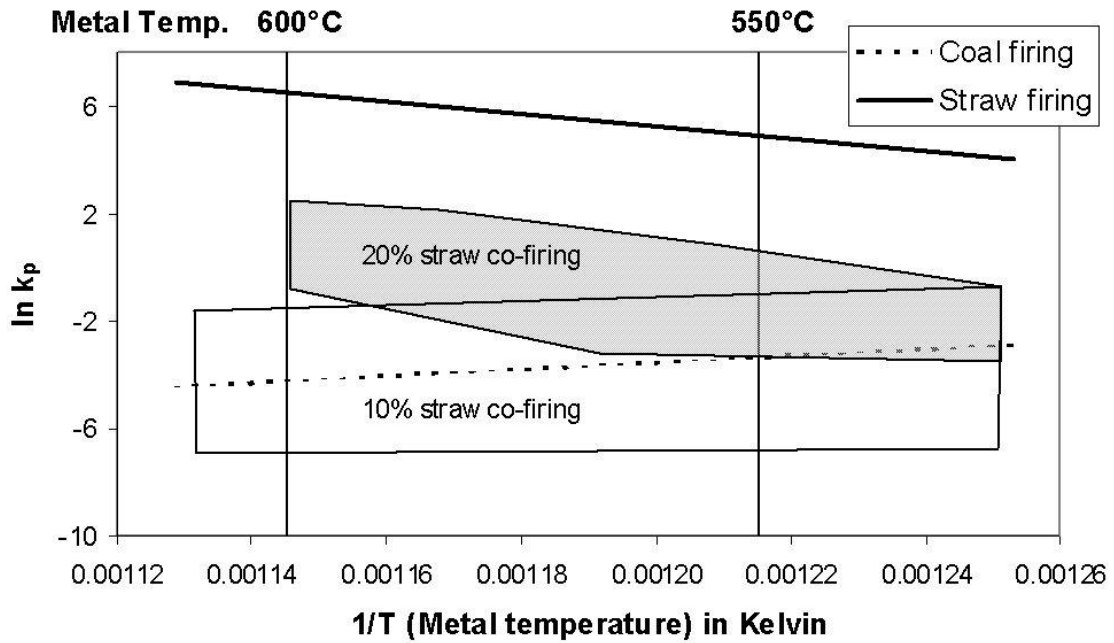
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Figure 1. *Arrhenius plot showing corrosion of TP347H FG tubes in co-firing of straw and coal compared to 100% coal-firing and 100% straw firing* **(Frandsen, Montgomery, & Larsen, 2006)***.*

The corrosion rates found for co-firing of 10% straw with coal after several years of exposure display increased corrosion rates compared with those determined during the short-term (3000 hours) exposure obtained during the Studstrup Unit 1 demonstration project (Figure 2). Long-term corrosion rates for 10% straw co-firing thus approach the short-term corrosion rates for 20% straw co-firing.
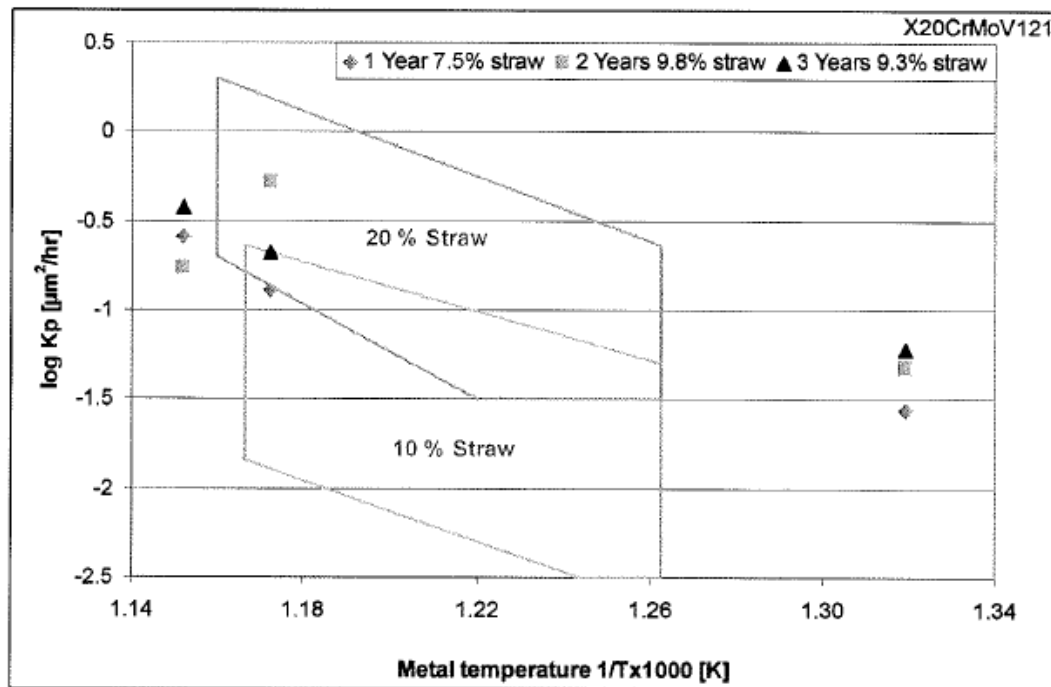
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Figure 2. *Arrhenius plot showing corrosion constant based on oxide thickness of X20CrMoV121 when co-firing straw and coal* **(Montgomery, Vilhelmsen, & Jensen, 2008)***.*

Corrosion rates for wood pellet + heavy oil + gas co-firing at Avedøre Unit 2 (AAV2) were similar to the rates seen for 20% straw + coal co-firing at Studstrup Unit 4. For detailed information on the tests and measurements at AAV2 is referred to report from: *PSO 6520 project: Corrosion measurements at AMV2 (Amager Unit 2) and AVV2.*

PSO 4788 was extended to include an overview on corrosion measurements at 8 different biomass and waste boilers of grate fired types in addition to the suspension fired plants mentioned. This overview is dated February 2009 and reported in Danish: *Afrapportering af Eltra PSO projekt 4788: Korrosionssamarbejde mellem Elsam, Energi E2 og IPL Materiale- og Procesteknologi.*

2.2   PSO 4766: Ash transformation

In sub-project 4788 (Corrosion collaboration) it was determined that the amount of aluminium and silicon in the fly ash decreases at increasing co-firing percentages while the amount of sulphur and potassium increases.
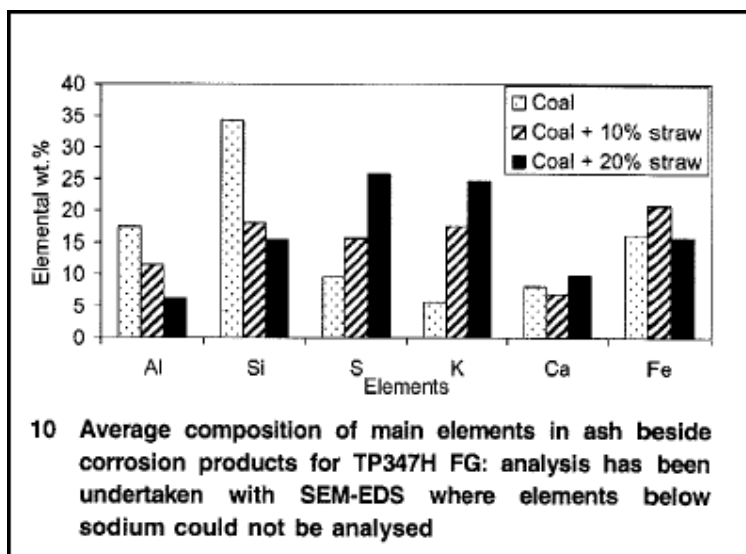

10   Average composition of main elements in ash beside corrosion products for TP347H FG: analysis has been undertaken with SEM-EDS where elements below sodium could not be analysed

Figure 3. *With an increasing share of straw, the amount of aluminium and silicon in the fly ash decreases while the amount of sulphur and potassium increases* **(Larsen & Montgomery, 2006)***.*

This corresponds to project findings based on entrained flow reactor tests where potassium and chlorine bonding with fly ash has been investigated (Figure 4 through). These tests show, that kaolin is an efficient absorbent of KCl from the gas phase. The absorption rate displays a minimum at around 1300°C. At this temperature, pores in the particle surface close while at lower temperatures, pore diffusion of KCl accelerates the absorption and at higher temperature diffusion takes place into a melted kaolin phase. Kaolin is present in appreciable quantity in coal fly ash and thus represents the properties of this. The significance of the findings is that the harmful gaseous KCl components in the boiler are absorbed by coal fly ash when this is present in sufficient quantity.
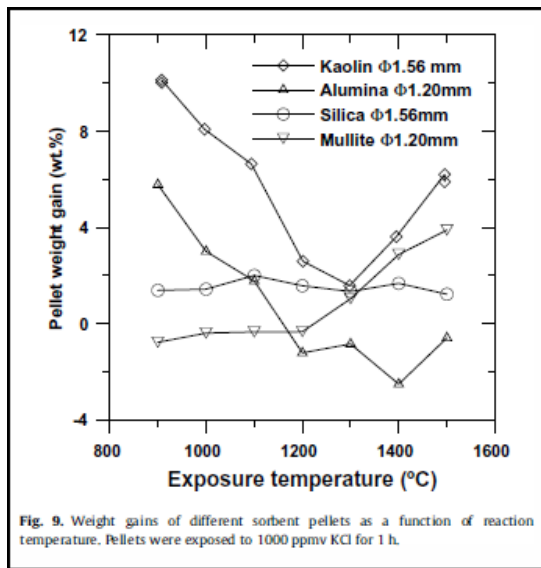
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Fig. 9. Weight gains of different sorbent pellets as a function of reaction temperature. Pellets were exposed to 1000 ppmv KCl for 1 h.
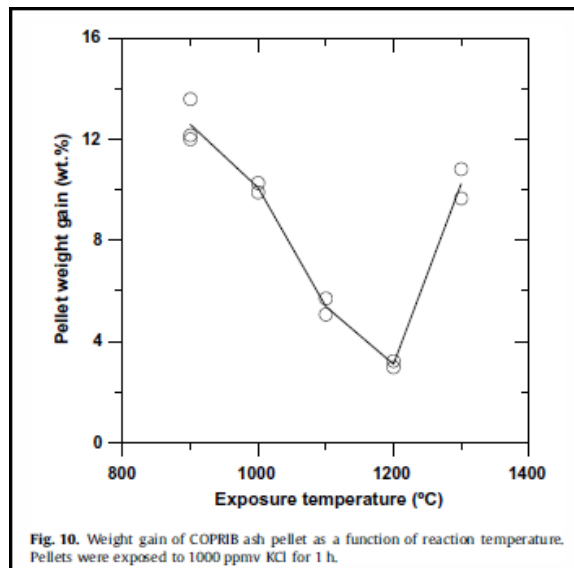
Fig. 10. Weight gain of COPRIB ash pellet as a function of reaction temperature. Pellets were exposed to 1000 ppmv KCl for 1 h.

Figure 4. *Kaolin which is found in coal fly ash is capable of absorbing significant amounts of KCl at normal combustion chamber temperatures.*

Based on the entrained flow reactor tests, rate expressions for the capture of gaseous potassium by kaolin pellets were determined (Zheng, Jensen, & Jensen, 2008). This result could be directly implemented in the CFD tools applied in sub-project 4805, where striation (channel formation) was investigated experimentally as well as numerically (see section 2.3).

Further details on the results from PSO 4766 are given in: *Final report PSO-Eltra 4766, dated November 2008.*

Fra slutrapport for PSO 4766 fremgår, at der er udført studier over sammenhænge mellem det samlede brændsels sammensætning og askekarakteristika samt af reaktion mellem gas fase KCl og diverse mineraler ved forskellige temperaturer.
I slutrapporten er kun antydet, hvorledes resultaterne eventuelt kan anvendes til CFD modellering af askeopførsel ved samfyring af kul og halm, men der er ikke udarbejdet algoritmer eller lignende der kan anvendes til CFD beregninger. Der er også formuleret et "blødt" forbehold ovenfor resultaterne: "It is important to realize, that the ash composition estimation is determined after the completed boiler processes, and also there are some significant uncertainties of the estimations."

Citater fra "response" fra DONG (til anden evaluering af 4105) dateret 6. oktober 2008:
1. I forbindelse med "Ash transformation":
"It is suggested that the development needs in this field be reviewed when projects 4766, 4788 and 4881 have all been concluded."
2. I forbindelse med "Enhanced deposit models":
"An improved generation of models have been implemented under both 4105 and 4881, but without the desired input from PSO 4766. There is no current initiative to include results from PSO 4766 into enhanced models, and it is suggested that the development line be reviewed when 4766 results are clear."

Spørgsmål: Kan der antydes noget om hvorledes disse temaer vil (eller bør) blive videre bearbejdet i det fortsatte F&U arbejde? CHEC har opslået en PhD annonce hvor kandidat søges til "PhD

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Scholarship in Fly Ash and Deposit Formation when Firing Biodust with and without Additives" som en del af GREEN projektet. Tilsyneladende som "forfra fra start"?

Bemærk, på AVV2 er der med succes tilsat kul-flyveaske som additiv til træfyringen for at undgå belægninger og korrosion, dvs. den additiv virkning kul har ved samfying er overført til ren biomasse fyring.

2.3   PSO 4805: Channel formation

One of the uncertainties of the exposure tests (deposition probes) performed was whether test elements had been exposed representatively. Co-firing of straw is performed with a high straw share on very few burners, and therefore it is difficult to ensure that the probe location reflects the actual (average) conditions. In practice, 10% straw co-firing (10% on energy basis) takes place by introducing equal amounts of energy input from coal and straw on four burners – i.e. 50% local co-firing ratio.

If the harmful components of the straw are not mixed evenly in the boiler right away, there is a potential risk that certain areas in the boiler experience a continuous exposure to hazardous elements which is much higher than the average at e.g. 20% straw co-firing. A measuring campaign was initiated to assess the differences of the 'local co-firing levels' in the combustion chamber around the first superheaters in the flue gas path.

A number of tests were conducted using different co-firing rates and boiler loads. During the tests flue gas and fly ash samples were extracted at different positions in the upper part of the combustion chamber.
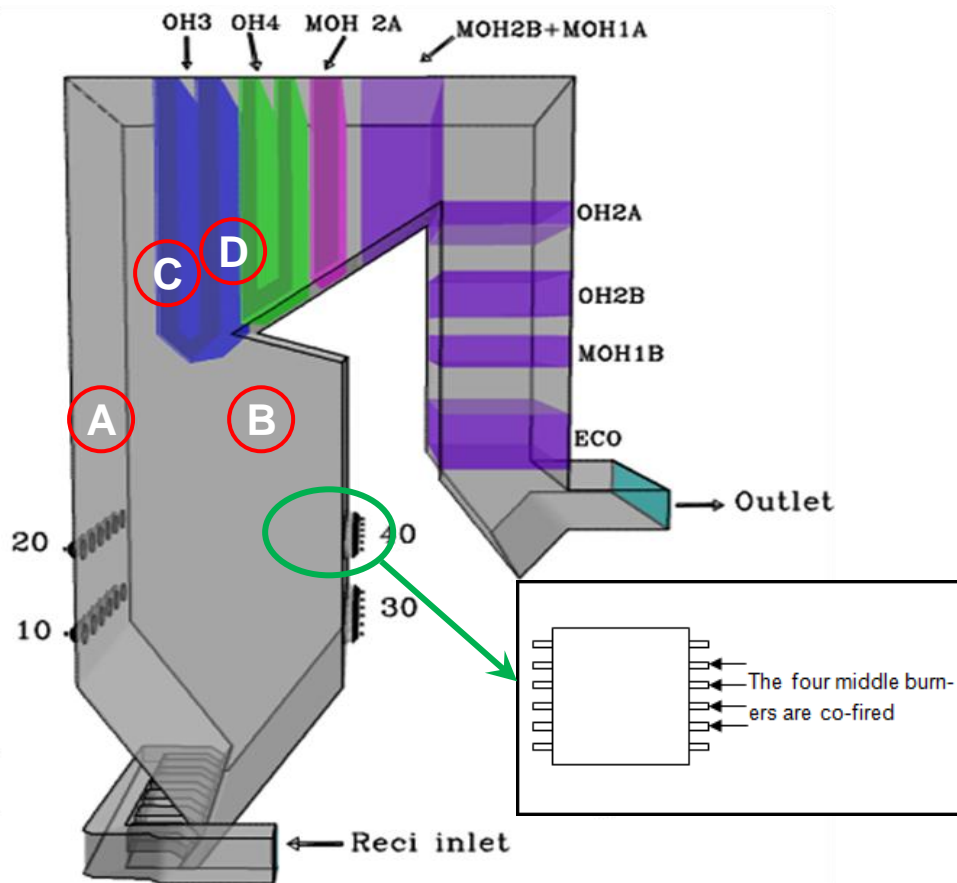
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Figure 5. *CFD model of Studstrup Power Station's unit 3/4 with location of sampling points A, B, C and D and indication of co-fired burners on burner row 40.*

The tests revealed that the concentration of gaseous components from the straw did not vary significantly between the individual sampling points. The particle extraction further showed that the share of unburned straw particles was largest near the wall opposite the co-firing burners. This observation was confirmed visually (Figure 6). The sequence of snapshots reveal that the inertia of the large straw particles prevents them from following the upward movement of the flue gas - instead they continue in a horizontal movement until they hit the opposite wall. Also, the large particles take longer to combust, which means that the share of carbonised particles from the straw is larger far from the burners.
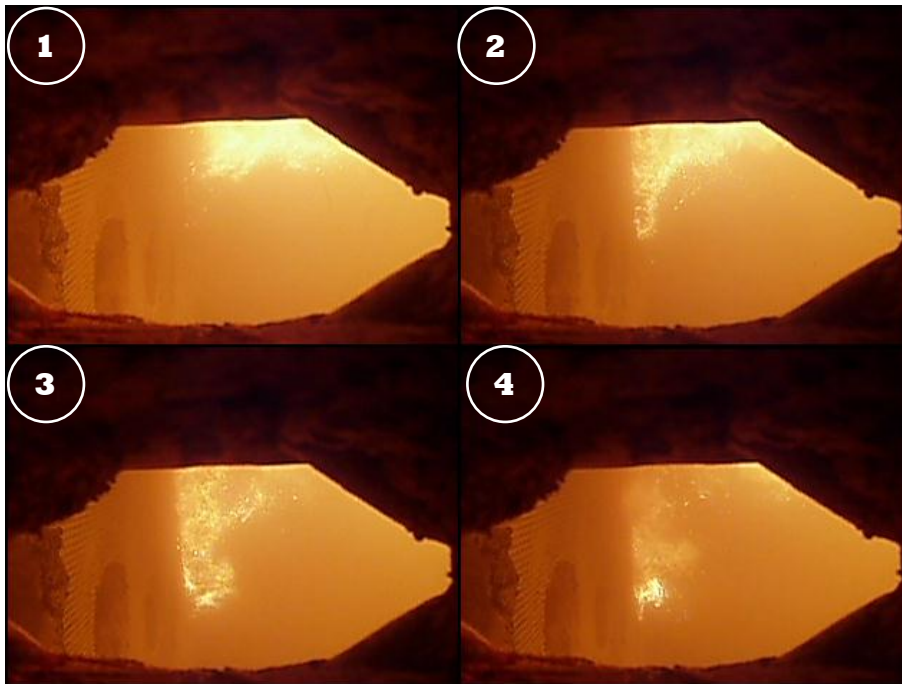
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Figure 6. *A view into the 13.4m wide combustion chamber of the Studstrup unit 3 boiler. Photos 1-4 show a burning 'cloud' of straw hitting the wall opposite from where the straw is introduced.*

The CFD modelling tool used for preliminary studies of straw co-firing in boilers was updated with the most recent results of the laboratory test of the KCl bonding in the coal fly ash as obtained in sub-project 4766. Simulations using the enhanced deposition model were performed to assess the rate of bonding within the boiler, and correspondingly in which areas there is a risk of the bonding not being complete.
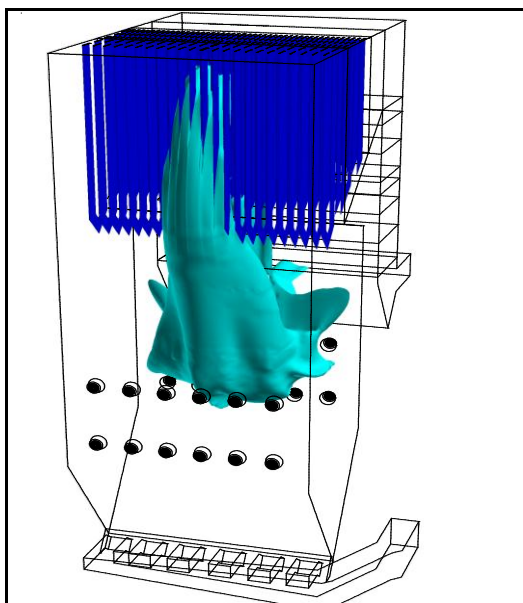

Figure 7. *Calculated ISO surface for KCl suggests that a full bonding of the potassium present in the coal ash is not obtained before the first set of superheaters. The rate of KCl bonding in fly ash may, however, be larger in full-scale than assumed due to the higher temperatures.*

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For detailed information on project results is referred to report from DONG energy: *PSO 4805 Final Report, dated January 2010.*

Bemærkning: I nævnte rapports afsnit 3.3 er beskrevet; "The data extracted from experiments and CFD simulations do not display very good agreement in the absolute values of species concentration". Dette bør nævnes i sammenfatningen (nærværende rapport).

Spørgsmål: Kan der skrives noget generelt ang, eventuelt videre arbejde på dette område, dvs. indenfor PSO 7333 eller GREEN projektet eller som et udestående tema for et nyt projekt?

2.4   PSO 4806: Low-NOx burner

The main emphasis of this project was the development of an improved CFD NOx model, based on the analytically reduced NOx mechanism formulated by (Pedersen, 1998). This NOx mechanism, and the CFD implementation of the model is termed the "LSP model". The main extension of this model to make it usable in a CFD framework was a methodology for estimation of radical pools from the major species solved for in CFD combustion computations.

Investigations carried out in a concurrent project (Damstedt, 2007) included mapping of local NOx concentrations in a $150kW_{th}$ laboratory-scale co-fired swirl burner. These data constituted the basis for comparison of calculations with existing NOx models implemented in Fluent® and the NOx model developed in this project.

The LSP model was verified against an extensive full-chemistry NOx mechanism (by Skreiberg, Kilpinen and Glarborg) for simple chemical reagents. If the LSP model is allowed to use the calculated radical concentrations from the complex model, it yields very accurate results for the formation and destruction of NOx. If the radical concentrations are based on equilibrium conditions with H2, O2 and H2O as developed in the current project, the accuracy of time development is reduced while end results are still accurate. LSP model predictions were far more accurate than existing models used in CFD (such as the DeSoete model).

The LSP model and radical estimation models were implemented in the CFD software Fluent®. Application of the model in a post-processing mode on combustion calculations performed for the laboratory reactor (BFR) shows that the model improves to some extent the trends that appear in the measured data, but also that the actual calculated NOx concentrations are overestimated. Existing models (De Soete) predict peak NO concentrations closer to measured values, but do not display the trends observed, see Figure 8 and Figure 9.

Bemærkning: Det foreslås, at der til sidst under PSO 4806 inkluderes en beskrivelse af eventuelle nye og fortsættende aktiviteter med at forbedre modellen. (Se senere bemærkninger)
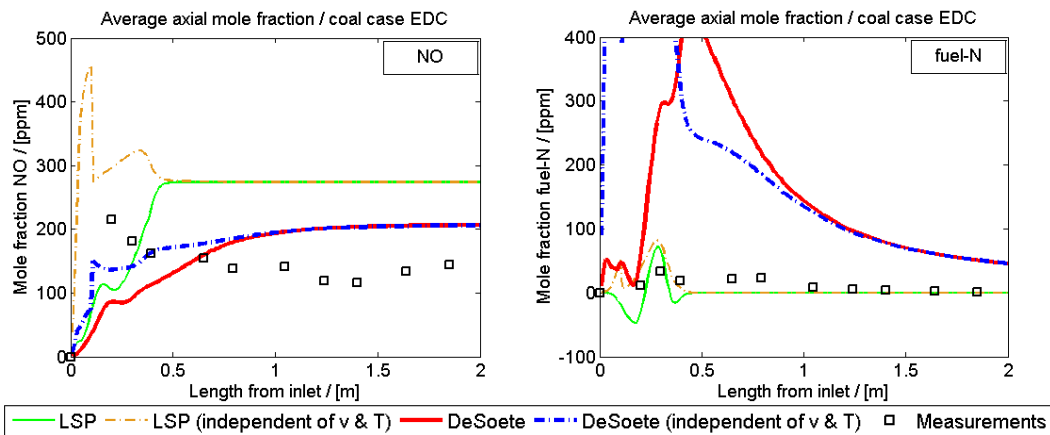
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Figure 8. *Mean concentration of NO and fuel N (HCN and NH3) in 50%/50% coal/straw co-firing.*
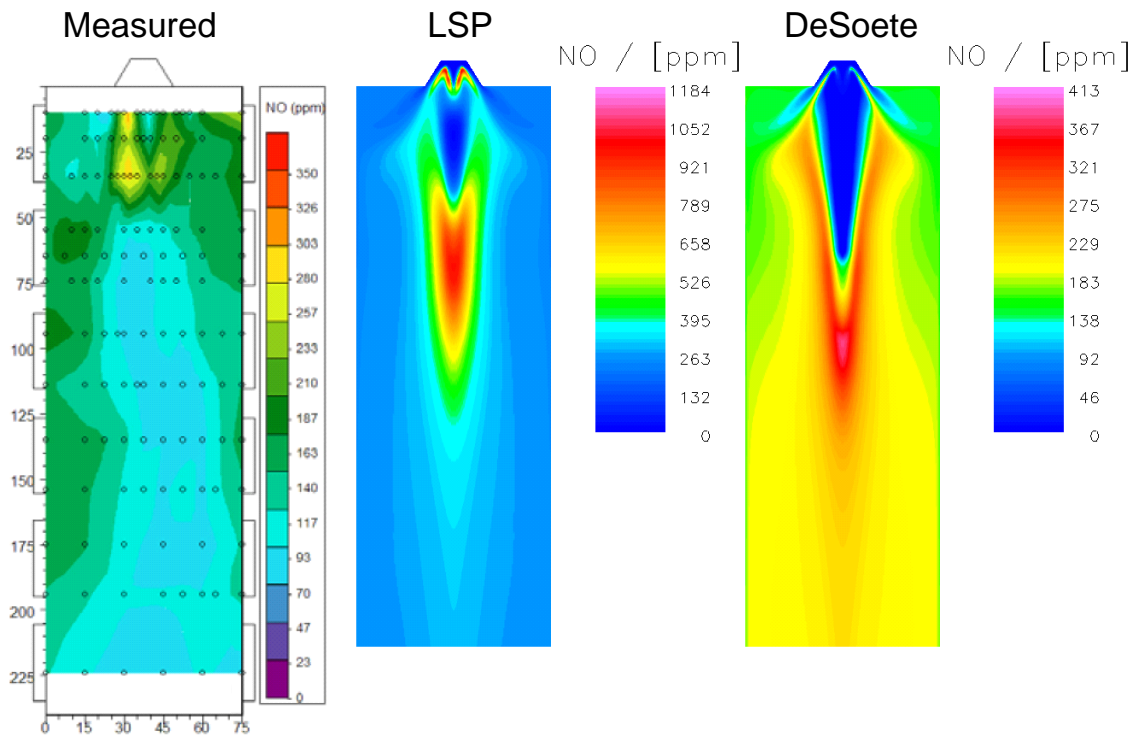

Figure 9. *Contour plot of NO concentration (ppm) in relation to coal/straw (50/50) co-firing. Measured data, calculated data using the LSP model and calculated data using the DeSoete model.*

Project PSO 4805 was split up in 4 tasks:
Task 1: Experimental characterization of NOx formation
Task 2; CFD-based NOx model development
Task 3: Chemical Engineering NOx modelling
Task 4: Low NOx burner modelling and design
For detailed information on the project results is referred to separate reports from each task.

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Bemærkning: Eventuelt kan den 1 sides oversigt: "PSO 4806 Report Overview", prepared by Søren Lovmand Hvid 4. November 2010, inkluderes i ovenstående. Det **er** meget svært at finde rundt I bilagene (totalt 560 sider), så en vejledning er nødvendig!

Spørgsmål: Er der copyright I forbindelse med nogen af rapporterne, så som Damsteds PhD (task 1)?
Bemærkning: Rapporterne fra task 3 og 4 er skrevet som om de skal indgå i et samlet skrift som henholdsvis afsnit 3 og 4. Det foreslås, at hver af disse rapporter får en forside. Rapporten fra task 1 bør også få en forside da den udgør Damstedts PhD uden projekttilknytning.

3.   PSO 4881 project status at project termination

A desired outcome of the PSO 4881 project was improved engineering tools capable of predicting the implications of co-firing on NO_x formation and deposit formation. These improved engineering tools were intended as CFD-based models, and the intentions were accordingly to improve existing models where these either had deficiencies related to the use of biomass fuel as opposed to coal or had general shortcomings which were desirable to improve.

The main deficiency of existing CFD models in the handling of biomass fuels relate to the particle size prominent in pulverized combustion of biomass fuels (straw or comminuted wood pellets). Existing particle conversion (or combustion) models treat particles based on two fundamental assumptions:
1. Particles are small enough to ignore internal gradients (thermal and/or composition)
2. Particles are spherical and thus geometrically describable by one parameter (diameter)

Both assumptions rest on assessments of typical particle properties that are violated in the case of biomass PF combustion, where particles are much larger than typical coal sizes (for which CFD particle combustion models have been developed) and also of quite different shapes than simple spheres. Both properties affect conversion times and hence volatile release rates as well as burnout rates. The volatile release is for obvious reasons extremely important when considering NO_x chemistry, as the entire combustion process depends on where volatiles are released and as the release affects local stoichiometry and temperature, which in turn is crucial in prediction of NO_x formation and destruction. For the same reason, the release of volatile components influencing deposit formation are just as important since the modelling of the fate of vaporised hazardous components will depend on where these components are released.

When the PSO 4881 sub projects were formulated it was clear that the particle sizes common in biomass PF combustion could not be handled satisfactorily by the existing particle conversion models. It was the intention to correct this deficiency by taking into account internal gradients within the particle when calculating release rates (moisture and volatiles). An extended model has been formulated and implemented in Fluent® (Yin, Kær, Rosendahl, & Hvid, 2010). Only further on in the project did it become clear that not only size effects but also particle shape had to be taken into account in the mathematical description of the conversion process if more complex chemistry such as NO chemistry was to be described with sufficient accuracy. This extension of the modelling complexity has been pursued in PSO project 7333.

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In the case of NO_x modelling, the work carried out during implementation of the LSP NOx model in the CFD code Fluent® (and in particular validation of the implementation) has revealed that there are some major challenges in this type of modelling, where the complicated NO chemistry modelling is decoupled from the combustion chemistry modelling (post-processed chemistry modelling):

- Since the NO chemistry is not handled concurrently with the particle conversion and combustion chemistry, heterogeneous reduction of NO on char cannot be included.
- The local oxygen concentrations (on a computational cell basis) determined by the combustion solution corresponds to the initial oxygen concentration in these cells – not the average or final. Since the NO chemistry is solved for based on this fixed oxygen concentration, the NO_x model uses a higher oxygen level than would be true since NO chemistry is much slower than combustion chemistry.
- Advanced chemistry/turbulence interaction models implemented in CFD codes are based on assessing the degree of mixing within a cell, or alternatively the degree of "active cell volume" taking part in chemical reactions. However, NO chemistry deviates from typical combustion chemistry in that it may proceed regardless of the presence of oxygen, and furthermore that the kinetic rates are highly dependent on fuel and oxygen concentrations.
- Species are known only on a cell basis and is consequently assumed to have this value in all parts of a cell. The computational cell (in the advanced EDC turbulence/chemistry interaction model) is divided into a "mixed" and "non-mixed" volume (with identical oxygen mass fractions) which is accurate enough for mixing-dependent combustion calculations. However, since kinetics are important in NO chemistry and as these are very dependent on oxygen and fuel concentrations, this approach is found to be insufficient despite the fact that the EDC model is able to incorporate kinetics.

The significance of all these details is that even though a much more accurate NOx model based on a validated, analytically reduced chemical scheme has been formulated and implemented, this model yields results that typically are further away from measured NO levels than current models. It is important to realise that this certainly does not imply that existing models are better or more accurate – this has indeed been shown not to be the case.

A suggested approach for the development of suitable turbulence/chemistry interaction model applicable to NO chemistry has been provided in the PSO 4806 sub project report.

A separate document named: "Biomass-Coal Cofiring: An overview of Technical Issues" has been worked out by Larry Baxter Brigham Young University, US and Søren Hvid, DONG energy .
In addition to the activities included in PSO 4881 the document summarizes contributions from collaborators in the US in the project and citations to related work from the global community.

Eventuelt bør der tilføjes noget om at PSO 4881 har "flyttet noget" i forbindelse med temaet "Biomass Cofiring", som dokumenteret i notatet, f.eks. i form af udvalgte citater.

4.   Conclusion

In conclusion, the PSO 4881 project has provided extensions of the existing model framework which resolves some of the model deficiencies that were acknowledged when the project was formulated.

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However, the modelling work carried out within the project has uncovered challenges in PF biomass combustion modelling which were not evident when the project was initiated.

These are related to:

- particle conversion (subject to treatment in PSO 7333 and in the GREEN project supported by the Strategic Research Council)
- NO chemistry CFD modelling, which has been pursued in other projects based on some of the ideas generated in PSO 4806 (Hansen, Stine, & Glarborg, 2010) (Hansen & Glarborg, 2010)
- A deeper understanding on issues and problems related to fly ash and deposits as experienced from plants running on bio-fuels (which will be studied in the GREEN project for dedicated biomass burners?)

Remark:
Søren Lovmand Hvids memo to the management of the GREEN project reveal a serious problem: Will the know-how accumulated in the 4881 and 7333 projects (and a series of earlier projects) be utilized in the GREEN project?

Citation from the memo:

4.2 Modelling

In context of the GREEN project, the objective is to support the development of dedicated biomass burners. Modelling tools based on fundamental rather than empirical description of physics are preferable in this task, as they allow much wider departure from conditions under which experimental data have been gathered. Since particle conversion is strongly influenced by "particle heat transfer history", which in turn is strongly influenced by burner aerodynamics, this points to the development of CFD-based particle combustion models rather than reactor network modelling tools. CFD models have already been formulated and to some extent implemented by other researchers as previously mentioned. It seems pointless to initiate a large initiative in this field within the GREEN project without taking advantage of this. We propose that the project management finds a way to exploit expertise in this field within groups not currently active in GREEN.

Remark: Clearly, the remarks from Lasse Rosendahl in context to the evaluation of the PSO 6364 project reflect the same problem: The new GREEN center will apparently not utilize the accumulated know-how and results from the PSO projects in a continued effort? Jeg læser citatet som at det drejer sig om ekspertice fra BYU (Larry) og AAU (Lasse).

Bemærkning: Et problem er selvfølgelig, at dokumentationen fra PSO 4881 projektet, der blev startet 2004, først er tilgængelig nu. Der er dog publiceret meget undervejs i form af en række artikler i tidsskrifter, konferencebidrag etc. Det er således ønskeligt, at der i nærværende "slutrapport" inkluderes en oversigt over alt det publicerede materiale samt de to PhD som "udbytte", dvs. en udvidelse af den allerede inkluderede referenceliste.

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