FLUIDIZED BED COMBUSTION AND GASIFICATION MODELING AND UTILIZATION OF THE MODELS FOR DIAGNOSTICS, CONTROL AND DECISION SUPPORT

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Abstract: In both gasification and combustion in fluidized beds it is important to keep control over the actual process and the sensors. In this paper models for both CFB and BFB for combustion, as well as gasification are described, and their utilization for different on-line applications described.
The mathematical models include the energy and mass balances for all relevant components. The dynamics is introduced primarily as change of temperature and chemical composition in a number of inventories. On line data is collected from all the sensors and a simulation is run to reach a balanced solution. The balanced values are compared to the original measured values and the difference between these is then plotted as a function of time for each variable. When the deviation is above a certain level a message is sent to the operators, that something may be wrong. This information together with other data is fed to a Bayesian Net, giving probabilities for different type of faults. In this way we get a diagnostics and decision support system that can be used also for maintenance on demand. When we have the dynamic modeled tuned we can use this to tune a MPC-controller. The MPC is run towards the simulator, and the response is used to develop the controller, instead of having to do a series of disturbances in the actual plant.

1. Introduction

In both gasification and combustion in fluidized beds it is important to keep control over the actual processes, to avoid sintering or blow out of bed material in the actual bed, or in the down comer G-valve. It is also important to keep control over the sensors. If the sensors are faulty, you may make the wrong control actions that may cause severe problems if you are on the boarder of what is acceptable with respect to economy and environmental emissions. Or you will just get poor performance generally, which may cause economic losses although less dramatically.

Malardalen University has been working together with power plants like Malarenergy in Vasteras and Eskilstuna Energy and Environment in Eskilstuna and vendors like ABB to develop models for both CFB and BFB for combustion, as well as gasification.

Malarenergy has a CFB for biomass combustion, 170 MW, and Eskilstuna Energy and Environment a BFB for biomass combustion, 95 MW. Malarenergy now is going to build a 200 MW waste gasification plant where the produced gas is going to replace coal in an existing coal fired PC-boiler. ABB developed a Black liquor gasification process using CFB (now Alstom power technology). All these processes have many common functions and thus we have tried to model them using a program Modelica, and then use this program for process performance monitoring, diagnostics and model based control.

If we now take a look at what has been done earlier in the area of data reconciliation we can mention some interesting papers like Crow et al [1983 och 1986], Sanchez et al [1992] and Romagnoli [1998]. Here methods for primarily steady state data reconciliation is presented and applications for chemical industries. Other methods and applications have been presented by Holst et al [2004] with a statistical graph-mixture method for fault detection, Wang et al [2001] a linear dynamic method applied for a refiner application, Latva-Käyry och Ritala [2005] using Kalman filters and moving windows and Avelin et al [2007] a combination of statistical and physical models. Applications for power plant applications have been presented by e.g. Avelin [2001], Karlsson et al [2004] och Karlsson et al [2007]. Terry and Himmelblau [1992] used an ANN method for data rectification and gross error detection in a steady-state process and Genrup[2005] applied an ANN method for turbine diagnostics in his PhD thesis work. Also Leibman et al [1992] were trying to do data reconciliation on dynamic processes, while they were using nonlinear programming techniques.

Concerning BN, Bayesian nets, professor Finn Jensen´s [2001] extensive handbook gives a very good overview of the technique as such. When it comes to applications for industrial use Weidl´s [2002] PhD-thesis gives examples from pulp and paper and metal industry applications on root cause analysis and decisions support on process operations and Widarsson et al [2004] gives an example from power plant operations on decision

support for soot blowing of super-heaters in a biomass fuelled boiler. Przytula et al [2003] also have made an evaluation of how BNs can be used for diagnostics in other applications. As background to the physical models we also can mention some papers of interest:

Bartusch [2002] Master thesis work on algorithms bed behavior and solids circulation for Boiler 5 at MälarEnergi AB. Bernard [1992] has made experimental investigation and numerical modeling of cyclones for application at high temperatures and Boysan and Swithenbank [1982] a fundamental mathematical modeling approach to cyclone design. Breitholz [2000] has made an extensive work on heat transfer in CFB-Boilers.

2. Model description

The mathematical models include the energy and mass balances for all relevant components. The dynamics is introduced primarily as change of temperature and chemical composition in a number of inventories. For the actual main fluid bed we have one, a second for the G-valve fluid bed and a third one for the steam system.

In this paper we describe the model and the utilization of it and the real life experience when the system is operated in the plants.

If we start with the basic functions of the fluidized bed processes, we can separate these into three main areas: fluid dynamics of particles in a gas flow, heat transfer, chemical reactions (combustion and gasification) and mass transport of reaction components.

Concerning the first area the fluid dynamics of particles in the gas phase we primarily can use simplifications of Navier-Stokes equations for this. As we have a two phase flow, and in the case of black liquor also the third, liquid phase, the solutions become pretty complex. When we try to add the chemical reactions and heat transfer, it becomes very complex, and in reality the problems have to be formulated in a more precise way for each single problem to solve. So, although we would very much like to have one single model, it cannot be achieved for the time being.

In our applications the focus is on diagnostics, and here the fluid dynamics at a micro level is of lower importance compared to the heat transfer and chemical reactions. The macro level of the fluid dynamics is influence the heat transfer and too low fluidization velocities can cause agglomerations, and these functions thus have to be included in the models. As the perspective is more “macro”, the mass transport of components (primarily diffusion primarily) can be treated in a more approximate way.

After defining these limitations, the mathematical equations have been limited to the flowing:

We are not only looking at steady state, but also on the dynamics of the processes. Thus we have included three inventories. These are for the gas/solid inventory in the boiler, the gas/solid in the G-valve in the case of the CFBs and the water/steam inventory in the steam drum and the circulation loops. There could be more inventories, but for our purposes these are the ones making sense to include.

The change of mass in each inventory for a time step then is described by:

$$\partial m_{inventory} / \partial t = \sum m_{i,in} - \sum m_{i,ut} \quad (1)$$

where $m_{i,in}$ is the mass flow of each component *i* and $m_{i,ut}$ is the corresponding out flow of each component *i*.

The change of the concentration c_i of each component *i* in the inventory we get from:

$$\partial c_i / \partial t = (\sum c_i * m_{j,in} - \sum c_i * m_{k,ut} - r_i * c_i * m_{j,inventory}) / m_{inventory} \quad (2)$$

where *j* is each flow to the inventory and *k* all flows out of the inventory. The chemical reactions are given by the third component where the reaction rate is given by r_i . The reactions can be both increase of e.g. CO_2 or decrease of e.g. C through gasification or combustion. The components addressed are C(s),H(s),O_2,N,S,CO,CO_2,H_2O(liq),H_2O(g),NO_2,NH_3,H_2S,SO_2,H_2(g), CH_4. For combustion only a minor part of these are actually needed. For combustion we assume that all reactions go to 100% from C,H,S to

CO2,H2O,SO2, while the production of NO2 is related to temperature and oxygen surplus (using a polynom). This is assuming more than 100% of relative oxidation. When oxygen is lowered in relation to organics CO is increasing using a polynom.

For gasification reactions we are using polynoms (PLS) produced from experiments made in a pilot plant for black liquor gasification. This is giving the gas composition of the product gas as a function of load, relative oxidation (e.g. 35% of the oxygen needed for 100% combustion of all organic components), % DS of the feed, pressure and reaction temperature. From these figures we then back calculate to get the energy and mass balances together.

The temperature $T_{inventory}$ in the inventory we determine from the energy balance:

$$\partial T_{inventory}/\partial t = = (\sum T_j * c_i * m_{j,in} - \sum T_k * c_i * m_{k,ut}) + \Delta H -$$

$$U*A*(T_{inventory} - T_{utsida})/ m_{inventory} *(\sum c_i * Cp_i)) \quad (3)$$

Here ΔH is the energy released during combustion, U the heat transfer number, A the area of the heat exchanger surface and T_{utsida} the temperature at the outside side of the heat exchanger surface.

The only difference between the BFB and the CFB is that in the BFB there is no recirculation flow of solids separated from the gas stream. There is no principal difference between the gasifier and the combustor, except for the difference in the chemical reactions. The cyclone separation efficiency is calculated using the stoke´s law for rotating flow (centrifugal force). From this we get the deviation speed in the radial direction (v_r/):

$$dv_r/dt = const* R^2*(\rho_{particle} - \rho_{gas})*v_\theta^2/r*1/\mu \quad (4)$$

Here R= the particle radius, $\rho_{particle}$ and ρ_{gas} the density of the particle respectively the gas, v_θ the rotational velocity in the cyclone and r is the radius of the cyclone. μ finally is the viscocity of the gas. The constant includes the shape effect of the particle as well as the effect of particles hitting each other.

The cyclone separation efficiency η now is calculated as

$$\eta = (dv_r/dt* \text{ residence time in cyclone})/ (0.5*r) \quad (5)$$

We assume that the average distance for the particles is half the radius, explaining the =0.5*r. The residence time is calculated as the (cyclone volume/gas_flowrate). Principally the separation efficiency is also affected in a negative way by flow rate gradients. We have not included it here but it could be described by $\eta_{corr} = \eta*(1-const*dQ/dt)$, where Q is the flow rate.

Still, there is a difference in the inorganic composition in the black liquor compared to the biomass combustion or gasification, and in reality the high amount of sodium salts in the black liquor is given a catalytic effect. Thus the reaction rate is significantly higher for black liquor compared to ”normal” biomass for a specific temperature, proportionate to the concentration of the inorganic content. This correlation is briefly given as a linear interpolation between ”pure wood” and typical black liquor.

A second limitation is the risk of agglomeration. For black liquor we have seen that the risk for agglomeration is increasing from 0.8 m/s down to 0.4 m/s, which is the minimum fluidization velocity. The risk is also at temperatures above 720 ^oC for ”pure black liquor”, while above approximately 850 ^oC when TiO2 is added.

For the selective absorption of H2S in relation to CO2 a separate model was developed for the scrubber. This includes both transport of gas to a liquid surface and different convections of gas and liquid depending on the scrubber design. With a low liquid mixing H2S will be rapidly absorbed, while the CO2 is building up high surface concentrations that will hinder more CO2 to be absorbed, as CO2 absorption is slow, and governed by kinetics and equilibrium concentrations. From the equilibrium concentrations we can see that an increased pH, that is reduced H+, will increase the absorption. By keeping the pH at 10.5 we can get a suitable absorption of H_2S but still reduce the absorption of CO_2.

$$K = [CO_2]\,[H_2O]/[HCO_3^-][H^+] \quad (6)$$

Diffusion of CO_2 as well as the reaction rate of CO_2 absorption is governed by:

$$\partial[CO_2]/\partial t = -D\,\partial^2[CO_2]/\partial x^2 - r*[CO_2] \quad (7)$$

Here we see that the CO_2 concentration in the liquid close to the gas surface is diminishing due to diffusion and reaction of CO_2 with NaOH and $NaHCO_3$. When there is a low concentration more CO_2 can be absorbed. By letting the liquid flow without convection the H_2S has been absorbed with a factor 20 higher than CO_2 in reality!

3. Results - utilization of the models for different purposes

Use for diagnostics

On a frequent basis like every 15 minute, every 2 hours or every 12 hours, data is extracted from the process data base for all the measured values of interest. The measurements are from all the sensors in the fluidized bed and the surrounding systems, but can also be complemented by lab-data or manual added information. These values are sent to the mathematical simulation model either as an average value or as a time series of values. In the first case we only want to find a steady state balance between different sensors to follow how sensors are drifting away, or permanent fouling is building up. In the second case we also can include the dynamics. The measured process data are introduced as initial conditions to the model, which then makes a simulation until a balanced solution is reached, using simultaneous solvers like DASSL (Differential- Algebraic solver) for the Modelica model (Dymola [Elmqvist et al 1995] or Open Modellica).

The typical measurements we have been using are: Bed temperature, temperatures at different positions in the exhaust gas train, feed water temperature and flow rates at different positions, steam temperatures at different positions, temperatures around the heat exchangers, fuel flow rate and estimated composition, concentrations of different components in the exhaust gas, MW_{el} and MW_{heat} produced and air flow rates.

The balanced, calculated values are now compared to the original measured values and the difference between these is then plotted as a function of time for each variable.

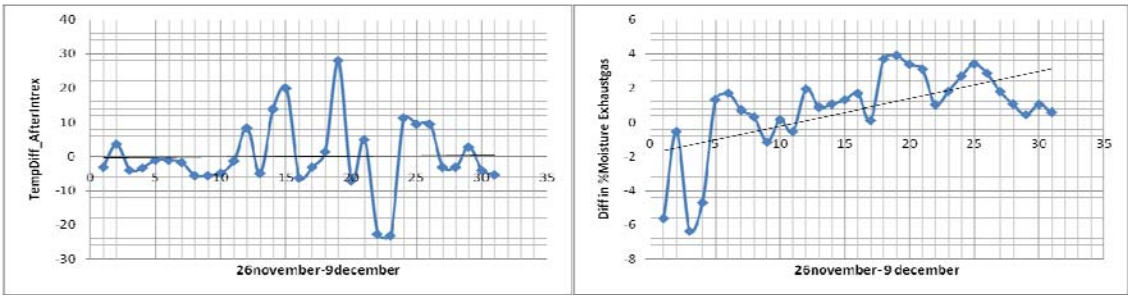

Figure 1: a) Deviation between calculated (balanced) and measured values for the steam after the Intrex in a CFB boiler (Mälarenergy). B) The deviation between calculated (balanced) and measured values for the moisture content in the exhaust gas in a CFB boiler (Mälarenergy).

By this we can see how differences in temperature measurements, gas composition, pressures and flows may be jumping up and down around an average values, or start to deviate upwards or downwards. When the deviation is above a certain level a message is sent to the operators, that something may be wrong. In Figure 1 we can see how the deviation in steam temperature after the Intrex (final super heater in a G-valve) is starting to oscillate in the middle of a period (a) while the deviation between the measurement and calculated moisture values in the exhaust gas is having a trend upwards during the same time period (b). This indicates problem in the Intrex fluidization or measurements in the first case, while either drift/fouling of the sensor or faulty assumed composition of the input fuel may be the cause in the second case (moisture or hydrogen content may be different).

This information together with other data like differential pressures over the beds, ash/bed exchange rate, variance in specific measurements like pressure measurements (clogging of the sensors is decreasing it) is fed to

a Bayesian Net which is giving probabilities for different type of faults. In this way we get a diagnostics and decision support system that can be used also for maintenance on demand. Tendencies for sintering in the fluidized bed, risk for irreversible fouling and other important process functions as well as sensor condition are included. Here we are using the known relations for risks for sintering or agglomerations due to high temperature or low fluidization velocity etc.

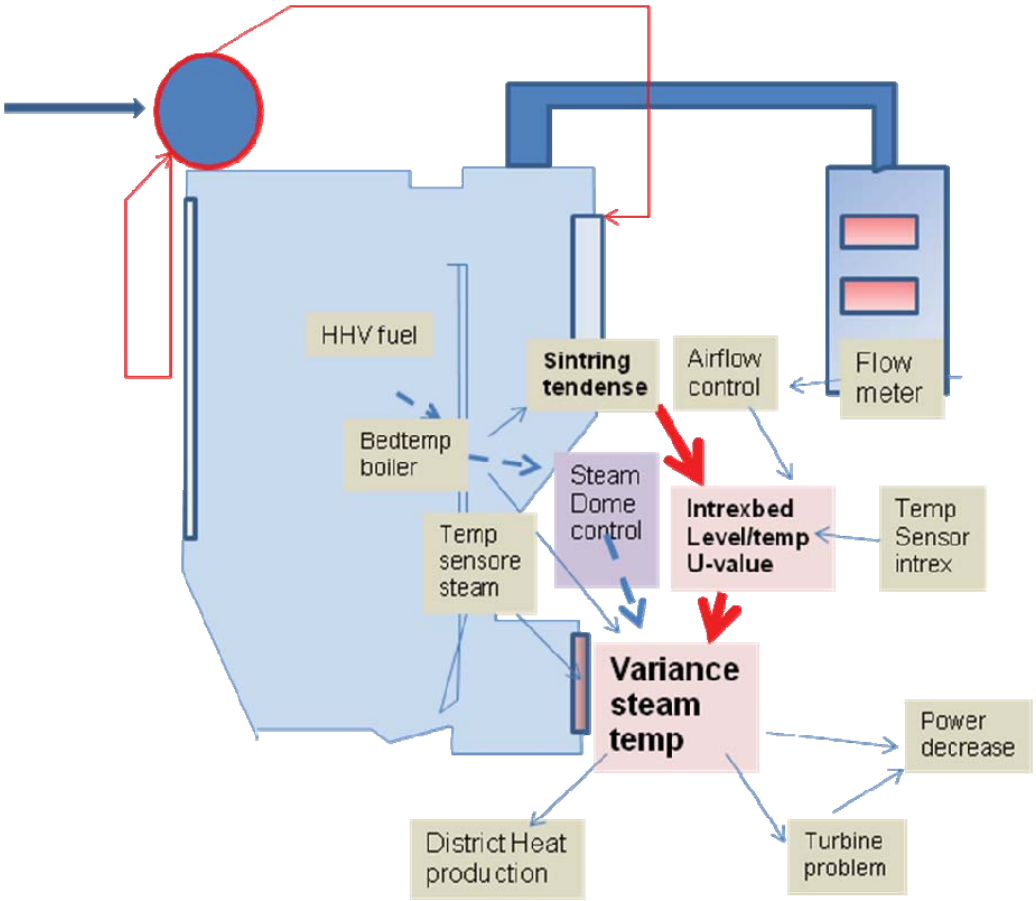

Figure 2 BN related to the high deviation in steam temperature after Intrex in the CFB boiler between calculated and measured values. Probable causes are seen in the arrow tree.

Use for Model Based Control

When we have the dynamic modeled tuned we can use this to tune a MPC-controller. The MPC is run towards the simulator, and the response is used to develop the controller, instead of having to do a series of disturbances in the actual plant. At least an initial tuning can be made in this way. This has been implemented at Eskilstuna Energy and Environment at their BFB boiler. This is described more in detail in Avelin et al [2009].

Use for design of new processes

One of the authors was project manager for the development of a CFB Black Liquor gasification project (originally ABB, now Alstom Power). Here we were dealing with solids with melting points from 450 ^{o}C and upwards. This means that we always have a certain amount of melts, but it will vary with both chemical composition and temperature, but not in a very clear way. Because of this it is very important to have a system that can diagnose the bed performance, to avoid agglomeration so that the bed collapses. One way of adding information is to actually listen to the noise caused by the bed. In the beginning we were just listening to the bed noise through a microphone/loud speaker, but this is really making you tired, so thereafter a diagnostic SW tool was used instead! By controlling the temperatures in the bed as well as around the G-valve and combining this with flow rates of air and fuel, we could determine the mass flow rate through the cyclone leg, which is key information needed. All this information together makes the input to the BN on risks for bed agglomerations.

The risk for sintering and agglomerations can be correlated to the amount of possible eutectics. If we for instance have 2 % KCl in the inorganic and 10 % Na2S we can form an amount of eutectic that is limited by the amount of the lower content component. In this case we can get (40+35 +(2*23)+32)/(40+35)= ca 4 % salt melting at the lowest melting point, approximately 450 ^{o}C. Sometimes it is reported in literature that the lowest melting point will cause a disaster, but this is not the case. Instead there is a need for a certain amount of melted components to keep the particles together in the FB.

From a principal point of view it would be good to inject the black liquor deep down in the FB and/or reintroduce dust collected in a bag house into the bottom of a bed and then let the particles attach to larger particles to build agglomerates. If this can be controlled in a good way, the particle burn out can be significantly increased. A not too small amount of liquid phase would then be positive, although the position of the melt in the particles also is of importance.

We actually were running with up to 4% KCl in the inorganic without any significant problems, and saw that the carbon content of the solids went down from 10 to below 2 % in the filter-dust when this was re-circulated back to the bed, while still below 1 % in the bottom ash.

A simulation model can be used to optimize the recirculation of dust in a full-scale plant.

From pilot plant experiments we collected a lot of process data. These were then used to make prediction models for the gas composition. In the figure 3 below we can see some results for the content of CO, H2 and residual carbon as a function of operational conditions.

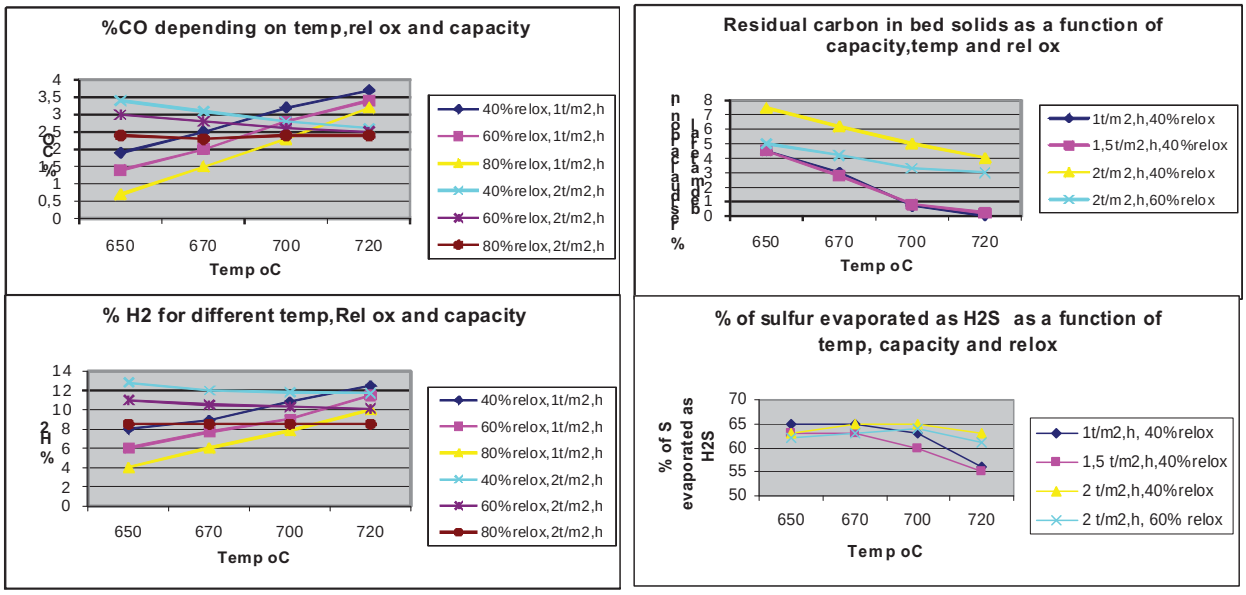

Figure 3 The content of different gas components (H_2,CO and H_2S) and residual carbon in the ash as a function of temperature, relative oxidation and reactor load with respect to black liquor (ton BL/m^2,h).

The gas composition is used to determine the final gas composition from the reactor. From this we calculate the theoretical energy and material balances for the processes, including also the additional processes with gas cooling, absorption of H2S and water in the scrubber etc. From this dimensional studies have been made where different alternatives like with and without TiO2 additions, different black liquor concentrations, different scrubber selectivity for H2S in relation to CO2 etc. Also different solids recirculation have been studied to get the right dimensioning data for filters, cyclones, scrubbers, heat exchangers etc.

4. Discussion and conclusions

What we have been showing in this paper is a method for determination of process performance in a way that is easy to understand and get an overview of for operators and process engineers. By combining mathematical models describing the physics of the process, and correlating different parts and functionalities to each other, more information can be gathered from the process compared to only studying a separate sensor as such. On the

other hand - by using a BN we can also include information from the specific sensors and even manual inputs of interest to get a diagnostic tool indicating the probabilities for different faults or process disturbances. This can be illustrated in an informative way by using cause tree structures, where the probable root causes of different faults can be followed in a graphical way. By following the evolution of faults the stability and accuracy of the predictions can be improved, and by including dynamics we can get a possibility to avoid some conclusions that are related to this, and are not “true faults”.

Acknowledgments

We thank VÄRMEFORSK and the Swedish Energy Agency for the financial support of this research, and Mälarenergy for support on the implementation.

References

Avelin A., Jansson J., Dahlquist E, “Use of Combined Physical and Statistical Models for On-line Applications in Pulp and Paper Industry”, *accepted Journal of Mathematical and Computer Modelling of Dynamical Systems 2007*

Bartusch Catrin: Bed Behaviour and Solids Circulation Algorithms for Boiler 5 at MälarEnergi AB. Diploma thesis work Mälardalens University, with Malarenergy. Västerås, 2002-11-03. Serial Number 2002-093

Bernard J.G., Experimental investigation and numerical modelling of cyclones for application at high temperatures, Delft university press, 1992

Breitholz Claes: Heat transfer in CFB-Boilers, 2000

Boysan ,F,W.H and Swithenbank,J,(1982),A fundamental mathematical modelling approach to cyclone design

Crowe C. M. : Data reconciliation – progress and challenges. J. Proc. Cont. 1996, 6(2/3), 89-98

Crowe C. M. : Observability and redundancy of process data for steady state reconciliation. Chem. Engng Sci.,1989,44,2009-17.

Crowe C.M., “Reconciliation of process flow rates by matrix projection. Part II: The nonlinear case”, *American Institute of Chemical Engineers Journal,* vol. 32. pp 616-623, 1986.

Crowe C.M., Campos Y.A.G., Hrymak A., “Reconciliation of process flow rates by matrix projection. Part I: Linear case”, *American Institute of Chemical Engineers Journal,* vol. 29. pp 881-883, 1983.

Elmqvist, H., M. Otter, and F. E. Cellier (1995): "Inline Integration: A New Mixed Symbolic/Numeric Approach for Solving Differential-Algebraic Equation Systems", In Proceedings of ESM'95, SCS European Simulation MultiConference, Prague, Czech Republic, pp. xxiii-xxxiv.

Genrup M., ”On Degradation and Monitoring Tools for Gas and Steam Turbines”, PhD thesis, Lund University, 2005, ISBN: 91-628-6470-X

Holst, A., Ekman, J., Gillblad, D., 2004, Deviation Detection of Industrial Processes, European Research Consortium for Informatics and Mathematics, **56**, 13-14.

Jensen, F.V., “Bayesian Networks and Decision Graphs”, Springer Verlag, 2001, New York, ISBN 0-387-95259-4

Karlsson C., Dahlquist E., “Process and sensor diagnostics - Data reconciliation for a flue gas channel”, Värmeforsk Service AB, 2003, (in Swedish).

Karlsson C., Dahlquist E. ,Dotzauer E.: Data Reconciliation and Gross Error Detection for Sensors in the Flue Gas Channel in a Heat and Power Plant, Proceedings PMAPS , Iowa, USA, 2004

Karlsson Christer, Anders Avelin, Erik Dahlquist: Improving the usage of process data collected in process industry and power plants. Conference proceedings Eurosim 2007, September 9 - 13, 2007, Ljubljana, Slovenia

Latva-Käyrä K. and Ritala R. Sensor Diagnostics based on Dynamic Characteristic Curve Estimation", 10th International Conference on Technical Diagnostics, Budapest, Hungary, June 9-10th, 2005.

Latva-Käyrä K., Ihalainen H. and Ritala R. Dynamic validation of on-line measurements: a probabilistic analysis. Submitted to Measurement, 2005

Latva-Käyrä, K. and Ritala, R., 2005, Dynamic validation of multivariate linear soft sensors with reference laboratory measurements. In: Kappen, J., Manninen, J. & Ritala, R. (eds.). COST ACTION E36, Modelling and simulation in pulp and paper industry, Proceedings of Model Validation Workshop, VTT Symposium, **238**, 57-64.

Leibman M. J., Edgar T. F. and Lasdon L. S. : Efficient data reconciliation and estimation for dynamic processes using nonlinear programming techniques. Comput. Chem. Engng, 1992, 16(10/11), 963-86.

Przytula K.W., Dash D., Thompson D., "Evaluation of Bayesian Networks Used for Diagnostics", Aerospace Conference, 2003, IEEE Proceedings, vol 7, pp 3177-3187, 2003

Romagnoli JA, Sánchez MC; "Data Processing and Reconciliation", Academic Press, San Diego July 1998.

Sanchez M. A., Bandoni A., Romagnoli J., "PLADAT – A package for Process Variable Classification and Plant Data Reconciliation." *Journal of Computers and Chemical Engineering* (suppl. 1992), pages 499-506.

Terry P. A. and Himmelblau D. M. : Data rectification and gross error detection in steady-state process via artificial neural networks. Ind. Engng Chem. Res.,1993, 32, 3020-3028.

Wang Y., Rong G., Wang S., "Linear dynamic data reconciliation : refinery application", *6th IFAC Symposium on Dynamics and Control of Process Systems*, Korea, pp 650-655, 2001.

Weidl G., "Root Cause Analysis and Decision support on Process Operation", PhD Thesis, Mälardalen University Press, 2002, ISBN 91-88834-36-0.

Widarsson B., Karlsson C., Dahlquist E., "Bayesian Network for Decision Support on Soot Blowing Superheaters in a Biomass Fuelled Boiler", Conference on Probabilistic Methods Applied Power Systems, Iowa, Ames, USA, 2004