Modelling and Simulation for Process Industry

VTT

Table of contents

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Modelling and Simulation for Process Industry

Modelling and simulation is a present-day way to understand and improve processes to meet increasing efficiency demands and maintain the competitiveness of industry. It has become an important enabling technology in decision-making, engineering and operation, covering the whole life span of a production line.

VTT has extensive experience (over 25 years of experience) in modelling and simulation for many industries. VTT offers a comprehensive set of tools and expertise for modelling and simulation of process and automation concepts: Powerful dynamic simulation with APROS, Conceptual process design with BALAS, Process chemistry with ChemSheet and Rotary kiln simulation with KilnSimu. These tools are ideal and useful for a wide variety of applications from steel mills to pulp and paper production, from energy production to biorefineries. Online and predictive simulation models can make you a forerunner in your business.

Benefits of process simulation

Using simulation-based methods to improve manufacturing has significant benefits. The benefits are achieved in terms of cost savings and intangible assets such as a deeper understanding of the process. The payback time of a typical improvement project is shorter than two years - in some cases only a few months. Benefits of applying simulation are:

- Reduction of capital cost by better design
- Reduction of time for design, commissioning, and start-up

- Reduction of pilot plant cost, size, and complexity
- Improved productivity and efficiency by material and energy optimisation
- Increased process knowledge and confidence in big decisions
- Training aid for new personnel
- Extension of equipment life
- Improved environmental management

Tools for process simulation

VTT offers a comprehensive set of tools and expertise for modelling and simulation of process and automation concepts:

- APROS - Powerful dynamic simulation
- BALAS - Conceptual process design
- ChemSheet - Process chemistry
- KilnSimu – Rotary kiln simulator

The use of models ranges through the plant life-cycle from off-line virtual unit operation and process concept design to the setup of on-line controls, training simulators and process development. In addition to simulation software and computational engineering expertise, VTT offers experimental facilities to complement demanding simulation studies.

Introduction

As tools of prediction, models can support thought and communication as well as training and instruction. They can be used for control or decision-making processes; to investigate complicated, expensive, dangerous, or inconvenient systems; to investigate systems in which study in real time would be a problem; to elucidate operating mechanisms for complex systems; and to investigate alternate strategies.

The modelling process may consist of the following steps:

- Recognition of a problem or an opportunity (in the current or new process)
- Delineation of the system to be studied
- Formulation of questions to be asked
- Gathering of the information *i.e.*, process and measurement data needed for the model construction
- Generation of the model (modelling)
- Running the model (simulation)
- Analysis of the results and their implications
- Defining how the model will be maintained for possible future needs

The usefulness of a model depends greatly on the quality of the model. A model must be simple enough to allow straightforward processing. Experience has demonstrated that the modelling of a complex system is most efficiently achieved by developing separate models for each part of the system. The parts are then successively linked together until the whole system is modelled.

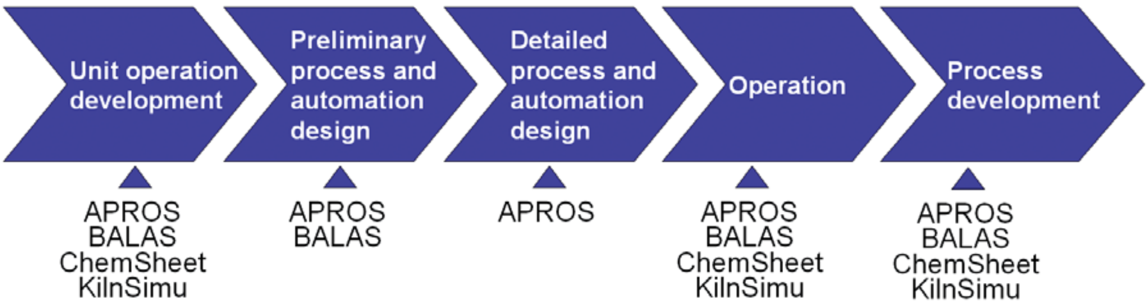
Simulation

A simulation model is a descriptive representation of the way a system operates. The model is intended for imitating the real operations in a virtual environment. Simulation involves first constructing a simulation model and then using that model to experiment with or optimize the performance of the system.

Process simulators come in various scopes and modes of operation. A general process simulator may be used to model the behaviour of a wide variety of processes, while a specific case simulator can be designed to predict the behaviour of a particular, well-defined process. Steady-state simulation is best suited for process design and optimization through generation of mass and/or energy balances. Steady state is an idealization of the behaviour of most continuous processes. Dynamic simulation is practical for tuning process control, start-up and shut-down scenarios as well as operator training.

The mathematical models employed by the process simulator generally consist of two parts. One part describes the properties of the materials that flow through the process and the other is for the behaviour of the equipment that exploits the properties of those materials. A major difference between property models and models of equipment behaviour is that property measurements may be made in the laboratory under controlled conditions. The measurements make it possible to generate data banks of chemical components and validate the physical and chemical property calculators in simulators. Unit operation libraries are used for constructing the behaviour of equipments. The operations of the system need to be matched with those in the library.

Simulation is extensively used in a situation when the real system cannot be used for experiments. However, there are also some limitations in process modelling and simulation. Naturally, the obtained predictions are only as good as the models and plant data available. Many process units might not have off-the-shelf equivalent simulator models. The physical and chemical properties of many substances might not be in simulator data banks or not accurately reproduced.



APROS® - Powerful Dynamic Simulation

The APROS simulator integrates process and automation design by offering a common platform for process and control engineers to demonstrate, discuss and further elaborate potential solutions. The simulator, once built in the design phase, can be directly reused in the testing of the real automation configuration. The interconnected process and automation system forms a very realistic and efficient system for operator training, both prior to start-up and after the plant commissioning. In daily production, APROS can be used for interactive problem solving and in improving control tunings or operational practises. APROS is developed and owned by VTT and Fortum Oyj.

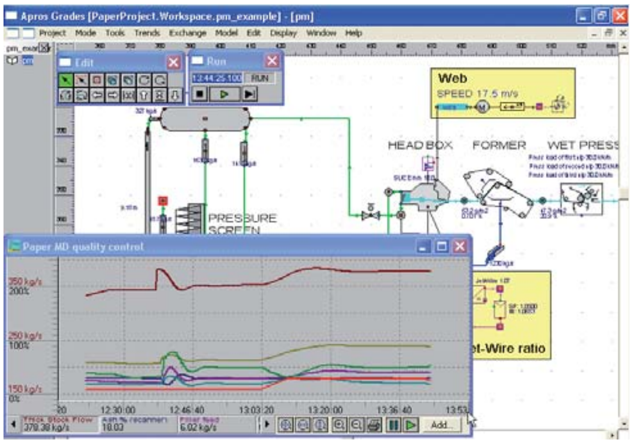
Customers

- Metso Automation built a training simulator for the Suomenoja power plant
- Metso Paper has used APROS to evaluate process and control design of new papermaking process concepts
- Fortum tested the automation system for the Estonian power plant at Narva using APROS
- APROS was used to perform the safety analyses of the Fortum's Loviisa nuclear power plant modernisation project
- A board machine of Stora Enso was modelled using APROS
- A SOFC fuel cell was modelled by Wartsila

Key benefits

APROS provides application oriented model libraries for full-scale modelling and simulation of industrial processes, such as Combustion Power Plants (APROS Combustion), Nuclear Power Plants (APROS Nuclear), and Pulp and Paper Mills (APROS Paper), all including gas/liquid flow networks, process automation, and electrical systems.

APROS promotes the re-use of model specifications made in the different phases of the process and automation life span: process pre-design, automation design,



detailed process design, planning of operational procedures, operator pre-training and re-training, analyses and optimisation and process revisions.

APROS simulation models are created and maintained graphically through the CAD-like user interface. The model is built up by dragging and dropping components from model library palettes, drawing connection lines, and entering input data using component specific dialog windows. The result is a P&I diagram with simulation specific additions, *e.g.,* the values of the calculated variables can be monitored.

The calculation is based on physical principles and empirical correlations. The fast and thoroughly verified network oriented solvers of APROS are table-driven, and accordingly, no programming, compilation or linking is needed during model development and simulation runs.

The openness of APROS allows the inclusion of user spcific models in the flow sheet as well as easy connections to external models, automation systems and control room equipment. APROS installations can be distributed and used in a local network by workgroup members. The extent of the applications can range from small computational experiments to models for full scope training simulators. The access in model data can be restricted to protect process design information *e.g.* in run time models.

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BALAS® - Conceptual Process Design

Process design and analysis is always based on the management of mass and energy balances. BALAS simulation tool is the most effective way to obtain information on the behaviour of an existing process and get a deeper understanding of the interactions in your process. Built-in link to MS Excel enables easy transfer and customised visualisation of simulation data. Model hierarchy, extensive unit operation, and chemical component libraries in connection with effective mathematical solvers make BALAS the solution for simulation of steady-state and tank dynamics, optimisation, and parameter estimation for pulp and paper processes. BALAS is developed and owned by VTT.

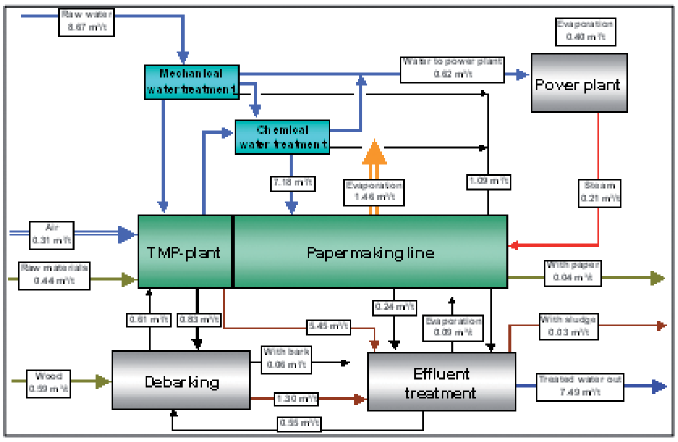
Customers

BALAS is used widely in the Finnish Pulp and Paper industry (m-real, Stora-Enso, UPM, Kemira, Andritz). VTT has extensive experience of concept studies in papermaking processes especially in the area of water management and energy efficiency. Over 40 papermaking processes have been modelled with BALAS. Half of them are energy efficiency and process integration studies and half water management studies. Consulting companies performing their studies with BALAS are: Papes Oy (part of Pöyry Group), Elomatic, AIRIX, Balance Engineering.

Key benefits

BALAS has an extensive selection of unit operation modules. These unit operation modules enable the user to model the whole paper mill including mechanical pulping, heat recovery, utilities and wastewater treatment. Selections of ready-made model processes, which are listed below, are supplied with the software:

- TMP
- PGWS (News)
- PGW-70 (SC, LWC)
- DIP
- Paper machine (uncoated)



- Debarking plant
- Effluent treatment plant
- Water preparation plant
- CHP power plant
- Multi-effect evaporator

BALAS simulation models are created and maintained graphically through the user interface. The model is built up by dragging and dropping unit processes from model library palettes, drawing streams connecting units, and entering input data using dialog windows.

BALAS simulator contains five calculation modes: Process behaviour with pre-defined model parameters can be calculated using simulation mode. Design mode is used when one needs to define unit model parameters based on known output values on *e.g.,* mill measurements. BALAS has a solver for non-linear optimisation problems. Optimisation can also be applied for parameter estimation problems where process model is fitted to measured process data. The fifth calculation model is dynamic simulation, which enable e.g. modelling dynamic behaviour of tanks and time delays caused by piping.

BALAS is connected to Microsoft Excel. The Excel-link allows stream and unit information to be sheared with an Excel spreadsheet. The Excel-link can be used for pre- and post-processing of results, sensitivity analysis, and even as a platform for creating user interfaces for models.

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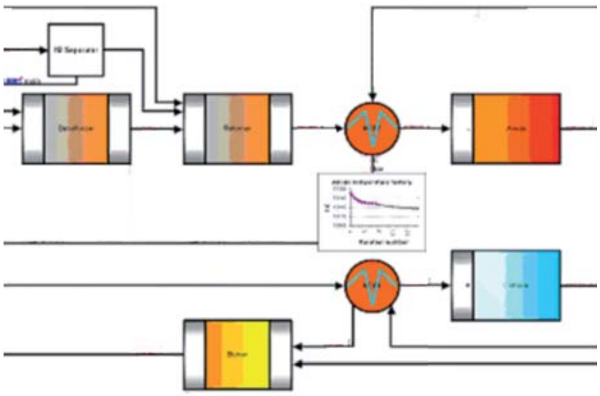
ChemSheet™ - Materials and Process Chemistry

Future models in process chemistry will increasingly be based on a multi-component, multi-phase Gibbs energy approach. ChemSheet is the foremost pioneer in Gibbs'ian process modelling. Taking advantage of unique immaterial constraints, ChemSheet handles reaction rate controlled chemical systems, multi-phase membrane systems, complex materials with surface phases, and much more. For example, in the multicomponent chemical theory of fibre suspensions, which combines the effects of ion exchange, Donnan theory, complex formation and precipitation/dissolution equilibria, the pH chemistry of pulp suspensions can be quantitatively interpreted. This opens possibilities for the use of simulation models for pulp and papermaking processes. ChemSheet capabilities can be combined into other software like the APROS, BALAS and KilnSimu, specialised in multi-phase rotary drums. ChemSheet is developed and owned by VTT and GTT-Technologies.

Customers

Chemsheet modelling is performed in various industry sectors and applications. ChemSheet is used for solving problems featuring the material choice, chemistry and the use of energy in complex practical systems. Some examples of the industrial applications of ChemSheet are listed below:

- Nuclear and energy engineering
- Fuel cell modelling
- Chemical reactor design, including scale-up and safety
- Dosage of chemicals in pulp bleaching and paper-making
- Environmental processing and effluent control
- Biofuel boiler design
- Design of pyro- an hydrometallurgical processes
- Inclusion control of steelmaking



- Surface science and material properties
- Reduction of carbon dioxide emissions

Key benefits

ChemSheet is a simulation tool that combines the flexibility and practicality of spreadsheet operations with rigorous, multi-phase thermodynamic computation. Customised applications are defined as independent worksheets in Excel and simulation are run directly from the spreadsheet application taking advantage of its functional aspects and graphical features. The models are connected to the thermochemical calculation routines through a plug-in component, which is created and maintained with a user-friendly dialog. When developing applications, writing macro-codes within the spreadsheet interface is helpful but for those who do not like programming, the custom made ChemSheet simulation model may appear as just another Excel file. ChemSheet was the pioneer of creating such a flexible interface to a scientific program, which since has become a must in the field.

Beginning with the additions of reaction constraints realised by the RateMix™ algorithm, VTT has pioneered in applying immaterial constraints to conventional Gibbs energy minimization. Within the international ChemSheet community a whole family of new multidisciplinary methods have emerged, their scope covering both practical engineering solutions and new developments in frontier sciences. Applications range from surface phenomena to high temperature material processing, from conventional process chemistry to environmental and geosystems as well as from the pH chemistry of pulp suspension to biochemical solutions.

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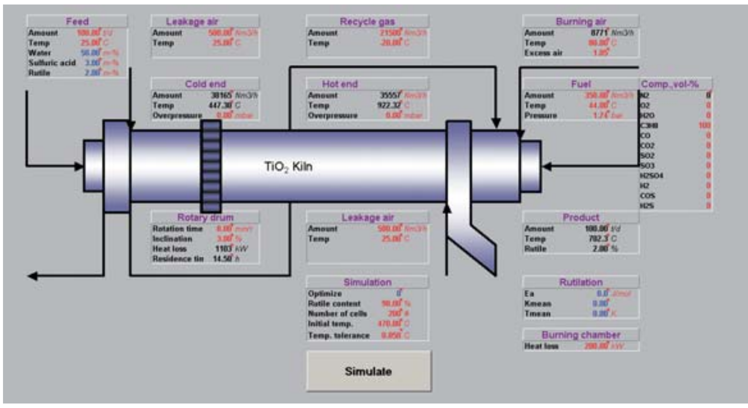
KilnSimu – Rotary Kiln Simulator

used in several industries. Though the technology of rotating drums has been available for over 100 years, it has not been replaced, but remains in active use in many of its traditional applications. The rotary drum provides an efficient means for both heat and mass transfer in the processing of slurries and other condensed mixtures.



Customer

Pigment and cement manufacturing industries are using rotary drums for the thermal treatment of various materials. In the chemical recovery of kraft pulping rotary drums are applied for lime recycling. Other uses are in the manufacture of oxides (aluminium, zinc, lead), reduction of ores and in waste incineration. Currently KilnSimu has customers in Finland, Japan and Italy.

Challenge

There is increasing interest in the complex chemistry of rotary drums, as many of the raw materials as well as the fuels used as heat sources vary in their chemical composition. This variation may lead to undesired emissions in the off gas or maintenance problems of the kiln. One common problem in lime kiln is the formation of rings due to alkali compounds. An additional challenge is created by the structure of the kilns. Due to the rotating cylindrical steel cover, the monitoring of the kiln interior is difficult. Due to long residence times, which may exceed 10 hours in continuous operation, undesired chemical pathways should be avoided. Thus it is often beneficial to use a reliable simulation model to depict and control their internal processes.

Solution

Most kilns operate in the counter-current mode, *i.e.*,, the condensed material is fed into the kiln from the cold 'feed end', and is then processed to reacted product by heat transfer from the surrounding hot gas, which is introduced into the kiln from its hot 'burner end'. The final material product is removed from the hot end. A fraction of exit gas can be circulated back to the hot end to improve the heat transfer efficiency. As a heat source, a fuel burner operating with the primary air is typically used. In KilnSimu the rotary kiln is divided into number of axial calculation zones, in which the radial temperatures of material bed and gas flows and inner and outer wall of the kiln are assumed constant. The volume elements of material bed and gas in the zones are described as open thermodynamic systems, which transform mass and heat with each other. The chemical composition of the volume elements are calculated by thermodynamics, yet taking into account the time-dependent mass and heat transfer between the elements and their surroundings. The kinetics of the material bed reactions are incorporated by dividing the solid phases into reactive and inert subsystems by using experimental reaction rates. The bed and gas flows of the kiln are calculated in a successive manner until all the energy and mass balances converge to an accurate solution.

Key benefits

The simulation yields axial temperature profiles for the bed, the gas and the inner and outer walls. In addition, axial phase compositions of the bed and gas flows are calculated. Results can be used to optimise fuel consumptions with different material feed capacities and to study the effect of using various fuels. Other uses are optimising the gas circulation and other energy factors including the kiln geometry. KilnSimu is also well suited for kiln scale-up.

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References

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Optimising Grade Changes

One of the leading paper and board producers Stora Enso Oyj wanted to shorten grade change time to improve productivity. An automatic grade change program was tuned using a dynamic simulation model of the board machine. Better understanding of the process was achieved and productivity was increased because of shorter grade change time.

Customer

Stora Enso Oyj is one of the leading paper and board producers in the world. This work was done at Imatra Kaukopää mill, board machine number 2. The board machine in question produces 3-ply packaging and graphical boards having a basis weight area of 170-350 g/m^2.

Challenge

Board machines produce tens of grades to meet different customer specific needs. To avoid large storage, mills have to change grades frequently. Grade changes (GC) have a large impact on the machine production efficiency, so it is relevant to make all possible efforts to minimize the production losses they cause. Typically there is at least one GC per day on the machine. For many years, a specific automatic grade change program (AGC) has assisted operators at the mill. However, the general feeling has been that the operation could be improved to give shorter GC times and to reduce moisture fluctuations during the GC's.

Solution

The decision was made to use a simulator to get a better understanding of the factors affecting grade change (GC) time and to optimise the tuning of the automatic grade change program (AGC). The accomplished process model covers the board making process from pulp chests to the end of the base board drying. The control system model includes 74 control loops. The model was built using the APROS Paper platform. The focus was on optimising AGC parameters that define the mutual coordination and rates of the ramps of the controlled variables. The simulator was validated against measurement data from real GCs on the machine. The number of reference GCs was over 50.

After confidence was gained that the simulator can consistently repeat the GCs that have been made in the real machine, the what-if experiments were started. Simulations concentrated on speeding up the GCs simply by increasing the ramping rates of those variables, which most often limited the total ramping time. One by one higher rates were experimented and the effects on the performance analyzed. After extensive testing with the simulator, the best set of tuning parameters were taken into production use on the real machine. The machine's GC performance was monitored before and after the changes and positive development was observed.

Key benefits

As a result the grade change time has been shortened by 10 -15% and the pay-back time of the simulation and optimisation project was 8 to 12 months. A procedure was developed to simulate grade changes and search for better AGC parameter values. It was no longer necessary to rely on intuition in the tuning.

During the work, undesirable operator actions in using the AGC, were noticed. After these faults were identified, the operators were advised asto the optimal and consistent use of the AGC.

It is a demanding task to figure out how the automatic grade change program (AGC) parameters should be changed to speed up grade changes and simultaneously maintain high paper quality. The simulator helped to cut the problem into pieces and offered a way to visualize the problem and compare the solution candidates.

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Advancements in Plywood Production Line

IMPROVING PRODUCTION AND ENERGY EFFICIENCY

Elomatic, a Scandinavian consulting and engineering company, started using BALAS process simulation software in spring 2008. Since then, simulation of mass and energy balances in small-sized as well as large process integrates have been performed. One of Elomatic's recent development projects was done for the Finnforest Plywood mill in Suolahti. The objective was to simultaneously increase both the capacity and the energy efficiency of the production line. With the simulation model, the current status and the effects of veneer dryer re-build on the energy efficiency of the mill were evaluated.

BALAS® Process Simulation Software

Customer

Elomatic is a leading Scandinavian consulting and engineering company and a global software provider. Nearly 700 Elomatic engineering professionals work within the paper & mechanical, process, energy and shipbuilding industries. Elomatic received a commission from Finnforest (a wood products company) to carry out an energy efficiency survey on the Suolahti plywood mill.

Challenge

In the plywood mill, the production was restricted by the capacity of the veneer dryer. The aim of the development project was to simultaneously increase both the production capacity and the energy efficiency of the mill.

Solution

A BALAS simulation model describing mass flows and heat exchange network (steam, condensate and hot water system) was built. The model was validated with the data collected from design parameters, automation system, stand-alone process meters and manual measurements. The model enabled several hundred options in terms of energy efficiency to be evaluated quickly. The best were selected for more detailed investigation.

Key benefits

The simulation model enabled the investigation of the effects of veneer dryer re-build on the energy and mass balances of the mill. The implemented veneer dryer re-build was chosen based on the simulation results. The built model can be utilized to evaluate future changes in the process. It also serves as an instrument for decision-making in investment projects.

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Controlling Process Chemistry

Co-operation with UPM in the development of process chemistry control in neutral papermaking was started as calcium carbonate $CaCO_3$ was introduced in mechanical pulp containing paper grades. Multiphase equilibrium calculations performed with ChemSheet have helped to quantify the acidification chemical and buffering aid at different stages of the process. Multiphase calculation combined into BALAS process simulation has given the customer a better understanding of bleaching practices in neutral papermaking.

IMPROVING pH AND CALCIUM CHEMISTRY CONTROL

ChemSheet™

BALAS™ Process Simulation Software

Customers

UPM is one of the leading pulp and paper producers in the world. Co-operation with UPM in the development of pH and calcium chemistry control in neutral papermaking began almost a decade ago when calcium carbonate $CaCO_3$ became a more common raw material in the production of mechanical pulp dominating grades. Unit operation studies have been performed for several paper machines as well as for de-inking and mechanical pulping processes. In recent years multiphase calculation has been combined into process simulation performed with BALAS software enabling monitoring the chemistry of large process integrates.

Challenge

Papermaking chemistry is vulnerable to changes in pH, temperature and ion concentrations as the behaviour of inorganic compounds and organic wood based compounds depend on these properties. Acid conditions accelerate the dissolution of $CaCO_3$. This leads to pigment loss and increases the amount of dissolved calcium and foaming. Fluctuating concentration of dissolved calcium induces unwanted inorganic and organic precipitation. Better process understanding and improved control practices were needed to minimise process chemistry variations in neutral papermaking.

In the beginning of the co-operation, the focus was on pulp acidification and pH buffering concepts. Lately, a pioneering chemistry simulation of a process integrate consisting of two paper machine lines with both mechanical and de-inked feedstocks was performed. In this integrate difficulties were often experienced when the bleaching dosages increased greatly according to the high brightness target of the paper.

Solution

The unit operation models of pulp acidification showed that when aiming to minimise $CaCO_3$ dissolution, carbon dioxide (CO_2) is a fair choice, if the pulp contains much $CaCO_3$ *i.e.*, de-inked pulp. Unit operation modelling was also used to quantify chemical dosages for pH buffering test runs.

BALAS process model of the integrate suffering fluctuations was complemented with the multiphase chemistry calculation and validated against chemistry data measured during the production of paper grades with low brightness target. Calcium chemistry in the production of the higher brightness grades was studied with the simulator.

Key benefits

The unit operation models have been useful in comparing different chemicals in pulp acidification and they have supported *e.g.,* the replacement of H_2SO_4 with CO_2. With the model quantification of pH buffering aid dosage, the number of test runs has been minimised. The simulations of the large integrate quantified the $CaCO_3$ loss at different stages of the process and a better understanding of bleaching practices in neutral papermaking was gained.

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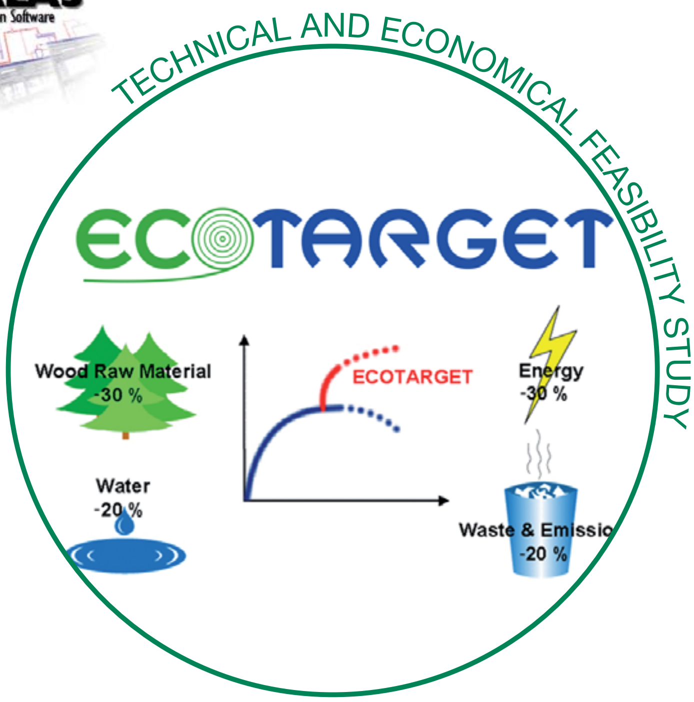
Evaluating New Process Concepts

BALAS process simulation software was used as the modelling tool in the evaluation work of new process ideas in the ECOTARGET project. Its flexibility for the wide range of new ideas and its capability in calculating the utility systems and mill level data for Life Cycle Analysis (LCA) were utilized in the project. BALAS link with MS Excel for post-processing purposed was utilized both in technical and economic evaluation.



Customer

ECOTARGET was the largest research project ever in the European pulp and paper industry. Leading universities, research institutes and companies in the field were participating in this project directed towards new and innovative processes for radical changes in the European pulp & paper industry.

Challenge

All ideas within ECOTARGET aimed at reducing the use of at least one of the four target areas: wood raw material, energy, water, waste & emissions. The challenge set was how to evaluate the direct goals given, as well as the technical and the economic performance of the ideas under development.

Solution

A decision was made to use BALAS process simulation software in the evaluation work of the different technologies under development in the ECOTARGET project. VTT, as the owner of the software, was able to provide the BALAS to be used during the duration of the project.

To be able to evaluate new process ideas, pulp and paper reference mills were first needed. These were selected and built as typical mills in different parts of Europe. In the next stage the evaluation models of the new ideas were built. BALAS is linked to MS Excel, which enabled the easy data post-processing. Mill level performances as well as the economic feasibility at the mill level were evaluated. The selected business scenarios were studied as well.
The models built consisted also of the steam and condensate systems including heat recovery systems, water circulation systems and air systems.

Energy costs have a dominating effect on the total cost of an integrate of mechanical pulping and papermaking. In the project, the fuels for energy production and electricity purchased from the grid were calculated as well as process steam from heat recovery and the required low and medium pressure steams from the power plant.

Mill level data was provided for further Life Cycle Analysis from harvesting to the end product. It consisted of air emissions, effluent information, raw materials, chemicals and primary energy need in the form of fuels and electricity.

Key benefits

BALAS is a flexible process design tool for concept studies and it was used to evaluate the wide range of new ideas in the ECOTARGET project. It was capable of providing the mill level data needed for test further Life Cycle Analysis from harvesting to the end product.

BALAS is linked to MS Excel, which enables efficient data post-processing. This feature was utilized in both technical and economic evaluations.

On the side of more conventional process calculations, BALAS provides rigorous utility system calculations for steam and condensate systems including heat recovery systems, for water circulation systems and for vacuum and ventilation air systems. BALAS is capable of providing effective calculation tools for power plant simulation, too, which were needed in calculating the primary energy consumption levels.

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Testing Automation with Simulation

Control and operation principles were designed and tested by utilising high fidelity full scope simulation before the commissioning phase. During the simulator testing several inaccuracies were realised. Without simulation it would have been impossible to notice these inaccuracies before start-up testing of the plant. Thus, the commissioning period was clearly smoother and faster.

APROS
ADVANCED PROCESS SIMULATION SOFTWARE

Customers

Foster Wheeler Energia Oy is a Finnish boiler supplier. In this project Foster Wheeler supplied a Circulating Fluidized Bed (CFB) boiler to Mälar Energi Ab, Sweden. Foster Wheeler used Process Vision as a partner to develop a simulation model for the new boiler.

Challenge

The design of an optimal control system to a power boiler plant is an extremely challenging task. Especially, if the process concept is completely or partly new to the manufacturer the control system should be carefully tested before the commissioning. Despite the clear need for thorough testing in as an early phase as possible the DCS-systems are traditionally tested in a full scope only with the actual process during the start-up period. Control circuit specific testing is not sufficient when the dynamical phenomena of the process have to be taken into account. This means that project personnel's valuable time in site is wasted in the testing and in the worst case the start-up of the plant is delayed.

Solution

In this project Foster Wheeler used the simulator innovately for control system application planning. This offered excellent possibilities to test the control logic with full-scale dynamical simulations before the actual DCS-control system was applied. The simulation system consists of DCS-emulator and simulation interface from Process Vision, CFB-model developed by Foster Wheeler R&D-centre and high fidelity APROS simulation system. APROS is an advanced dynamic process simulator developed by VTT.

The process modelling team of Process Vision used the same system and the whole system was tested including the challenging combination of the parallel steam lines of the new natural circulation boiler and the older once-through boiler to the sliding pressure turbine generator. Also the preliminary controller tuning and adjusting of various set point curves and other parameters were accomplished with the simulator. Simultaneously, the system offered unique opportunities for operator training well before the commissioning period of the new boiler. Since the simulator was utilised during the control application planning, it was possible to use a complete copy of the DCS-system in the operator training even though the actual DCS-system was not available.

Key benefits

"The utilisation of the simulator before the boiler start-up has offered remarkable advantages in operator training and in adjusting and testing the main control circuits. The operators have been extremely motivated during the training period due to the chance to be able to take part in this task. We have also obtained a great benefit from the training period thanks to the realistic GRADES Trainer simulator system of Process Vision and professional training personnel of the boiler supplier". - Jan Westin, Project Manager, Mälar Energi Ab, Sweden

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Innovative Boiler Design

Increasing use of biomass and waste mixes as fuels in boiler combustion creates new opportunities for clean energy industries. Yet, the wide variety of fuel chemistry with numerous corrosive agents brings also new challenges in boiler design. Metso Power's novel expert system, based on VTT's ChemSheet, overcomes these difficulties and gives a fair competitive edge and economic reward to its developers.

ChemSheet™

Customer

Environmental and climate concerns as well as increasing econ omical pressure on fossil fuels have increased the interest in biomass and waste combustion for power production. Benefits for Green Power generation also encourage the take-up of forest residues, urban and industrial waste, agricultural residues and sludge for producing municipal heat and electricity. The wide variety of such fuels and fuel mixtures requires quantitative tools for optimization of the combustion parameters, boiler design and superheater materials. For such needs, the STEAMAX expert system was developed by Metso Power [Sonja Enestam *et al,* Clearwater].

Challenge

The biomass and waste fractions are burned typically in boilers, which apply fluidised bed combustion. For fractions too difficult to burn on their own, co-combustion of various mixtures is applied. However, in such mixtures the contents of alkali metals and chlorine are frequently high, often in combination with sulphur. The presence of these elements easily triggers operational problems such as corrosion, fouling and bed sintering.

Solution

The chemical analysis of the fuel mixture together with the thermal conditions of the boiler superheater serve as inputs for the STEAMAX system. The expert software is a tailor made routine based on VTT's ChemSheet. The calculation gives the equilibrium composition of the burning mixture and the flue gas in the boiler conditions. The corrosivity of the fuel is then correlated with the chlorine and sulphur compounds of the mix and with the alkali composition of the ash. The index of corrosivity is estimated at different temperatures and locations in the boiler. Additionally, the risk of molten phase corrosion can be evaluated by the calculated ash melting curve.

Key benefits

STEAMAX is used in Metso Power for determination of the maximum steam temperature and for selection between acid-proof and low-alloy steels in the superheater. With the required steam temperature set, STEAMAX can find the optimum fuel mixture for the boiler, *e.g.*, the maximum allowed chlorine in the waste fuel. The STEAMAX corrosivity index supports the boiler operators in the choice of suitable fuel mixtures avoiding costly trial runs.

STEAMAX has been verified with Metso's long term experience from a large number of full scale biomass and waste boilers with good reliability. It has been successfully used in the design of several new boilers and boiler re-builds. While a typical superheater pack is constructed of ca 500 tonnes of steel, significant earnings can be won in reducing the consumption of up-scale construction material. The procedure with its complete reproducibility provides confirmed competitive advantage for its developers in Metso Power.

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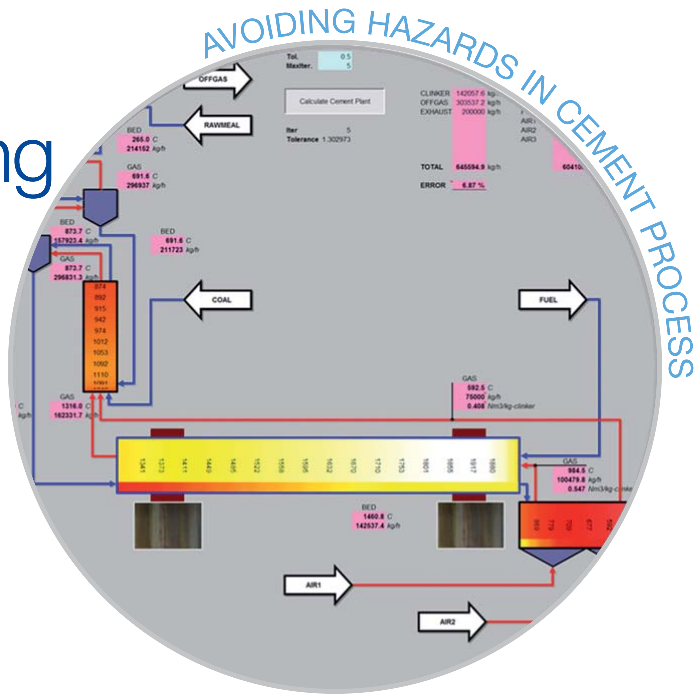
KilnSimu Model for Cement Manufacturing



Cement manufacturing is one of the most widely used industrial processes involving a rotary kiln unit operation. Cement process has two main variations: a wet process and a dry process. In the wet process a suitable mixture of raw materials is fed into the rotary kiln in the form of slurry which may have water content of 30 to 40%. In the dry process this "raw meal" is first dried with exhaust gas from the rotary kiln and then heated in a precalciner system typically consisting of several cyclones and riser duct that is fuelled with coke to calcine the limestone. Cyclones collect dust from the kiln's exhaust gas and that are mixed with partially calcined raw meal which is then fed into the kiln at about 800 °C. The advantage of the dry process is its lower fuel consumption and thus it is the main choice for cement manufacturing today.

Customer

VTT has provided Ube Industries, a Japanese cement manufacturing company, with a KilnSimu model for rotary kiln and clinker cooler unit in the dry cement process. Ube Industries has three cement factories in Japan with combined production capacity of nine million tonnes of cement a per year. Ube Process Technology Research Laboratory has combined KilnSimu with Aspen® flowsheet model to describe the whole cement manufacturing process.

Challenge

There is an increasing interest towards using alternative fuels in the cement process as additional heat sources and for waste incineration in the rotary kiln and the riser duct. Typical candidates in the Ube factories are waste plastics (including pachinko panels), oils, tyres and even tatami mats! These additional fuels may have a high content of volatile elements like such as sulphur and chlorine which react with alkali metals to form sulphates and chlorides. These then accumulate in the process through alternate vaporisation at the hot end and precipitation at cold end of the kiln and in the cyclones and cause cyclone clogging, ring formation, and accelerated brick damage in the kiln.

Solution

KilnSimu cement model contains a full thermodynamic description of the phases and species in the cement system. These include gaseous species, liquid slag and solid solutions and around 100 pure solid phases. The mixture of raw materials consists of calcium carbonates, silicon oxides, aluminium oxides and iron oxides occurring as limestone, sand, clay, bauxite, laterite, *etc*. In the precalciner most of the calcium carbonate is first calcined to calcium oxide or lime at 800-900 °C. Then in the kiln lime reacts with other raw materials at 1200-1450 °C to form calcium and iron silicates and aluminates that are the main components in the burned product called cement clinker. A special version of KilnSimu was prepared with a clinker cooler unit which is used for cooling the clinker from the rotary kiln and also for preheating the air going into the kiln and the riser duct. The cooler is typically a grate kiln where air is blown from the bottom of the cooler through the grates and the clinker in a cross current fashion.

Key benefits

KilnSimu model was successfully used to predict the cement clinker crystal formation and composition and to estimate the circulation of sulphate and chlorine species in the precalciner and rotary kiln. Results can be used for making a correlation between the brick damage rate and the behaviour of sulphates and chlorides.

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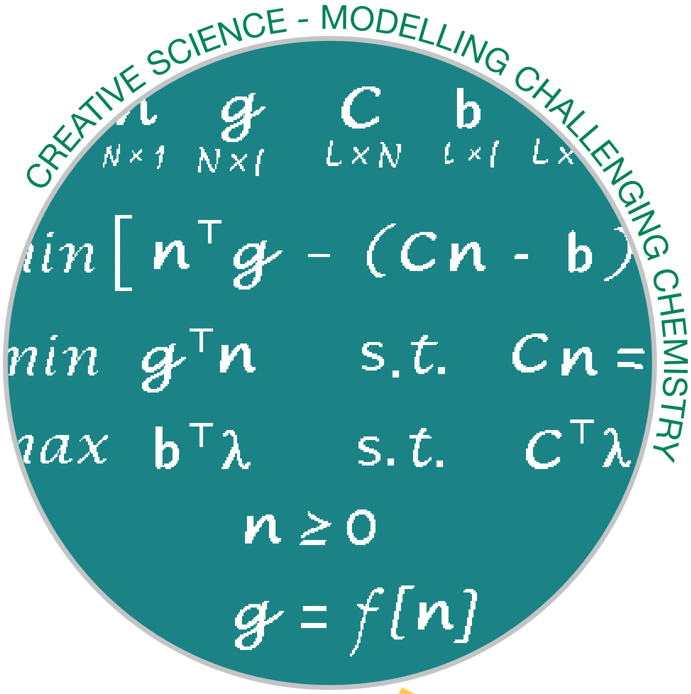
Advanced Chemistry



Energy is one of the most important concepts used to describe the physical and chemical behavior of systems. Mathematical modeling based on energy is successfully used to computationally investigate interesting chemical changes.

Customers

This method is intended for researchers and scholars trying to understand the behaviour of Gibbs energies in a chemically reactive system. Its use will aid in determining the dynamic control structure and the physicochemical responses to various alterations. The method is applicable to materials science, geology, pulp and paper, process chemistry, organic chemistry, biotechnology, and chemistry in power generation. New computational implemantations and theoretical advancement is performed as required.

Challenge

Systems containing large sets of reactants and their possible reactions lead to a lot of work if every reaction needs to be screened and parameterised experimentally. It becomes more elaborate as the number of possible phases and phase combinations increase. Together, the number of reactants and phase combinations can become so large that the system behaviour changes too rapidly for the experiments to make sense. Experimentally testing random alternatives in search of some optimised property may become too laborious and may hinder the endeavour.

Solution

This method uses Gibbs energy minimisation to determine the relative order of magnitude of time constants for a set of chemical changes. This information is achieved indirectly by generating the sets of chemical changes that are comparatively instantaneous, comparatively unattainable, and those that are the rate limiting factors at some pertinent conditions.

Gibbs energy minimisation uses an entity conservation matrix to describe physical and chemical constraints. Given a set of instant or rate limiting chemical changes, a suitable conservation matrix can be generated by a new systematic procedure, which creates an entity balance matrix augmented with the proper reaction constraints for the rate limiting chemical changes. Physical energy contributions that affect the chemistry may be incorporated into the mathematical model by enlightened changes to the entity conservation matrix, when multidisciplinary investigations are desired. Theoretical advancement or computational development might be needed to model novel sets of chemical changes.

Key benefits

Creating a mathematical model of the system directs the creator into finding the important aspects of the particular system at hand. Numerically explicit models enable computation of selected variables that can then be compared to experiments for validation. The more elaborate a model, the more variables can be calculated from a smaller set of parameters. Although the modelling is an educational journey, the resulting model may be used to computationally probe the possible behaviour of the system at different conditions. A similar approach may be used to find correlations between parameters and to determine the sensitivity of the calculated variables.

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Future Concepts


Picture is courtesy of Metso Power Oy

BIOFUELS

Increasing uses of biomass and waste as fuels in power production or as feed for syngas production create new challenges for ash chemistry and emission control as well as for process operation. The corrosivity of fuel mixtures will require particular attention from both equipment manufacturers and operators. Advanced simulation tools such as ChemSheet, APROS and Balas are used to support boiler manufacturing and operation.

OIL REFINERY – BIOREFINERY

During the last decade, utilisation of sustainable biomass and biotransformation processes has spurred increasing interest. The number of commercial processes producing biomass-based chemicals and biofuels is growing. VTT is among the world leaders in developing biomaterials and 2nd generation biofuels, with a main focus on non-food and forest based feedstock.

The new era of Biorefineries will require advanced process simulation techniques covering both thermal and hydrolytic routes in processing biomass. Thermochemical multi-phase techniques will also appeal mineral oil practices when facing increased amounts of brines and condensates.

Picture is courtesy of Wartsila Finland Oy

FUEL CELLS

VTT is developing a research infrastructure to support industries' fuel cell activities. This includes the building up of know-how and human resources, experimental facilities and computer models, using APROS and ChemSheet as tools. Examples range from 20 kW SOFC to small printable micro fuel cells. At present, VTT is developing methods for the production of hydrogen and hydrogen-rich fuels for fuel cells by reforming hydrocarbons as well as gasification and advanced gas cleaning.

NUCLEAR SAFETY

VTT is a forerunner in the development of nuclear safety expertise and advanced nuclear technologies. Customers have access to the expertise and network of the whole of VTT and its modern experimental facilities and modelling tools such as APROS and ChemSheet.

VTT performs contracted research on challenging topics related to nuclear safety, plant life management and nuclear waste management. In this way VTT maintains comprehensive, up-to-date know-how, computer code systems and experimental facilities for the safety analysis and operational support of nuclear power plants and waste management facilities.


Picture is courtesy of Fortum Oyj

More information about these concepts

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