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SIMULATION STUDIES OF A CALCINATION KILN PROCESS

M. Ketonen*, K. Penttilä , P. Koukkari

**Kemira Engineering OY, on the leave to:*
Hunter Timber Ltd,Old Golf Course Site, Fishtoft Road,Boston PE210BJ, UK
fax : + 44-1205357550
VTT Chemical Technology, P.O.Box 1404, FIN-02044 VTT, FINLAND
email: pertti.koukkari@vtt.fi; karri.penttilä@vtt.fi

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Abstract

As automation level of a processing plant is increased, careful consideration should be given to the development potential that novel devices offer to operate the plant closer to its optimal operating point. New advanced controls may be developed with the aid of computer based systems and modern measurements. These facilities also make possible the implementation of more advanced control and optimisation algorithms.

Simulation studies give insight to process phenomena that affect to the state of the process. Both first principles approach and “black-box”- modelling may be appropriate for different uses.

In this paper the economical motivation of a simulation study is evaluated for a calcination kiln process. A static first-principles model and a dynamic “black-box” model for the same process are shortly presented and their use in improving the operation of the plant is discussed.

1 Introduction

As automation level of a plant increases the assessment of future automation investment tends to become more nebulous because the improvements tend to produce benefits that are not easily calculated in monetary terms. The uncertainty of the expected future income may be treated with an uniform way by studying the its stochastic nature [1]. Still, numerical information about the expected behaviour of the process is needed.

When an automation level improvement is realised some credits may be found from the decrease of maintenance costs, increased availability of the plant and optimisation of the workforce. Such savings may have justified investments earlier but as the automation level rises the investments tend to become more strategic. Some tools are still needed to present the intangible benefits that are known to exist but whose quantity is unknown.

If no development of the actual process operations is not included in the investment the potential that the novel instrumentation and automation devices give is not used to the full [2,3,4]. The cost of the development work is often relatively small when compared with the expenditure of the new equipment.

In this work simulation techniques are used to get insight to a calcination kiln process. This is central part of the titanium dioxide pigment production process. The process is highly energy intensive, has high material throughputs and recycles. Its time constants range from few minutes to several hours.

The modelling work tends to produce benefits of different natures. The end-user of the model or simulations may develop her knowledge about the process. Even simple dynamic models may be used for on-line process control. The model builder herself tends to get most insight to the process during the modelling work. The goal of the modelling work has to be considered carefully when the basis and the structure of the model are determined. Different aims and users lead to different approaches to the modelling problem.

For static simulation the rotating kiln is divided to several “slices”. In each “slice” the heat balance is calculated and the advancement of reactions in the titanium dioxide phase is evaluated by minimising the Gibbs energy in the sub-system. The balances in all the “slices” are calculated successively. The overall heat balance is determined by iteration.

A simple dynamic model is presented for this process. It has been developed directly from process data. The static model can be used in the design of the process experiments as well as in the interpretation of some experimental results. The dynamic model is used for evaluations of the profitability of proposed automation investments. It is also used for evaluations of the effects of changing kinetics found by static simulation to the control performance of manual operation. A model incorporating control structure is presented.

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2 Process description

Calcination kiln processes described in Fig. 1 are widely used in titanium dioxide production, based on so-called sulphate technology, to produce dry crystallised titanium dioxide pigment from titanium dioxide slurry.

In this process the slurry is fed into a large, slowly rotating kiln where it is dried, heated and crystallised into a desired crystal form. The titanium dioxide phase is heated with a counter-current hot air flow. In the inlet end of the drum the temperature is above 300 ^oC and the outlet the product reaches temperatures above 900 ^oC. The energy is consumed by the drying of the slurry and the heating of the material to the point where the exothermic crystallisation reaction takes place. Then a crystal form changes in a desired degree to another form. The content of the desired crystal form in the product should be controlled evenly.

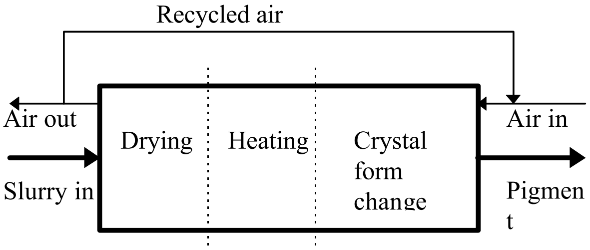

Fig. 1 A schematic diagram of the calcination process

Because the outlet temperatures are rather high the material tends to sinter. This is not desired since the product has to be milled to the size little over that of a single crystalline. If sintering occurs the energy needed for milling increases dramatically.

To save energy, some of the used hot air is recycled to the outlet end of the kiln. These large recycles decrease the stability of the system. The outlet temperature of the air is also limited due to the durability of the air scrubbing system through which the air is vented.

In this case the same equipment is used for different grades of pigments. These grades may have a significantly varying reaction kinetics caused by different pre-treatment of the slurry.

The range of the time constants is wide because titanium dioxide material and air have very different residence times in the kiln. The initial effect of a temperature change in the air inlet may be seen in few minutes but the total change to a new stationary state may take twenty hours. The changing kinetics and slowly changing states make the control of the process very difficult. Obviously, the temperatures in the air inlet and outlet are strongly interconnected.

The relationship between the crystal size and crystal form is important. Both factors affect to the product quality and in some cases it is very difficult to produce a product where both factors are in specification. In those situations it is advantageous to be able to drive either factor as close to its limits to be able to bring the other factor into the specification. This decreases the need for the post-treatment.

3 Economic motivation

Calcination forms an important part of titanium dioxide pigment process based on the so-called sulphate method. In calcination the titanium dioxide pigment changes its crystal structure that forms the basis for the most important quality factors of the eventual product. Because this unit operation is also very energy intensive the costs of the continuing research are justified.

The benefits of automation matrix (BAM) may be used to classify the expected benefits of an automation investment according to their technological background and the confidence level of their actual realisation [5].

The technological improvement may be sought in five areas: instrumentation, basic automation devices, advanced controls, plant information systems and information integration (Fig. 2). The benefits may also be described as hard, soft or intangible credits [6]. Hard credits are those that may be calculated on the basis of the improvements in the proposed investment and base case data [2]. The calculation of soft credits has to be based on experience from earlier projects in similar processes and environment.

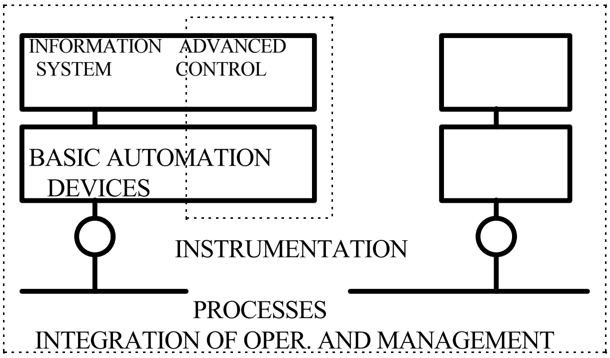

Fig. 2. Classes of technical improvements in automation investments

Intangible credits are those that are generally agreed to exist but are difficult to assess in monetary terms. These benefits may rise from various sources such as raised motivation of the plant operation personnel, good-will caused by enhanced environmental protection or market advantage from improved quality.

This research aims for improved control operations - weather manual or automatic- of the process and can therefore be considered to be in the “advanced controls” class. On the other hand the benefits may be caused for example by improved closed loop control that increase the capacity of the plant (hard credits), energy savings from more even control of the temperature (soft credits) and improved quality (soft credits). BAM in Table1 illustrate the areas where the benefits of this research are expected to be found.

Table 1 The expected benefits of simulation study of the calcination kiln process

	Hard credits	Soft credits	Intangible credits
Instrumentation			
Basic automation devices			
Advanced control	Increased capacity Less recycled material	Energy savings	Improved quality Faster reaction to upsets Improved insight
Information systems			
Information integration			

In this particular plant the instrumentation and basic automation devices have been recently upgraded. According to Fig. 3 this kind of investments should be completed by using the development potential that the modern equipment has. The full utilisation of the new devices both presupposes and facilitates thorough investigation of the process.

Table 1 represents the expected benefits of the modelling work alone. More benefits may be found when simulations can be used to predict the improved performance of the system if new measurement or sampling devices can be used. This is discussed shortly in chapter 5.

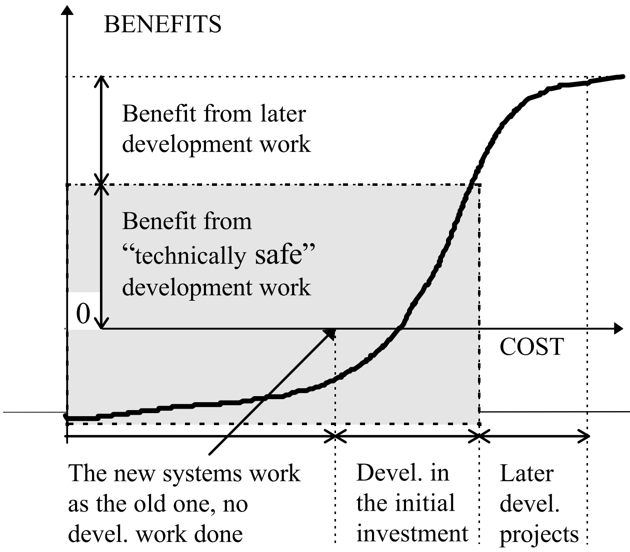

Fig. 3. Typical benefits versus investment cost for an automation level improvement project

The future work includes simulation studies that can be used to develop ideas of future control development projects and to evaluate the magnitudes of the possible benefits of such work.

4 Static simulation

4.1 The RATEMIX® Method

The RATEMIX® algorithm is designed to combine multicomponent thermodynamic calculations with reaction kinetics and heat transfer by using the *image component method* in Gibbs energy minimization. The introduction of image components to the thermochemical calculation procedure allows one to combine reaction rate theory with multi-component thermodynamics and the resulting models can be applied to simulate complex chemical reactors with simultaneous mass and heat transfer.

The reactors are calculated via *intermediate thermochemical states*, for which also the Gibbs energy and other state quantities become defined. The algorithm of the image method is described in Fig. 4.

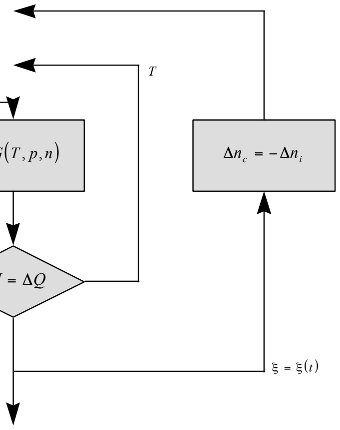

Fig 4. The calculation algorithm for the intermediate states.

In Fig. 4. the inner loop performs the enthalpy iteration which determines the temperature of the intermediate state. The outer loop controls the extent of the desired reaction as the amount of the image component (subscript i) becomes replaced by the actual component (subscript c) by finite differences. The increment is deduced from the overall reaction rate.

The method is applicable in systems where the salient thermodynamic and kinetic data are known and the time-dependent heat transfer data can either be measured or estimated by calculation. The simulation can be done for either stationary or transient chemical systems.

4.2 The Counter-Current Rotary Kiln

In this work, the RATEMIX® procedure was used to simulate the calcination of acidic titanium hydrate in the stationary operating rotary kiln.

The wet slurry enters the kiln at ambient temperature and the calcinated rutile TiO_2-product reaches temperatures above 900 °C. The drum is heated by a propane burner. The three reaction zones of the kiln are schematically shown in Fig. 5.

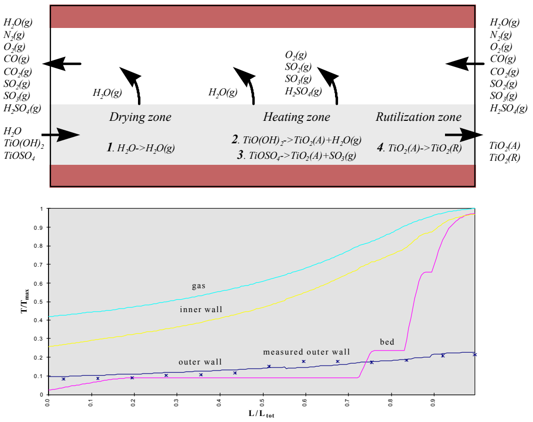

Fig. 5. The three reaction zones and the calculated temperature profiles of the titanium hydrate calcination. The dots indicate measured outer wall temperatures.

The simulation model was constructed to calculate the stationary temperature profiles of the kiln. To achieve this the kiln was divided to 100-200 successive "slices", in which the heat and mass transfer was assumed to occur in the radial direction. Axial heat transfer was neglected.

Further it was assumed that no axial mixing occurred in the reaction mass or in the gas. An axial plug flow model was used for both gas and the slurry. To take into account the effects of the physico-chemical transformations on the enthalpy balance of the reactor, the gas and the condensed mass were both described as thermodynamic systems. The main components of the gas phase are N_2, O_2, H_2O, CO_2, CO, SO_2, SO_3 and H_2SO_4, and the condensed phase is respectively a mixture of water, sulphuric acid, hydrous titania $TiO_2 \bullet nH_2O$, titanium sulphate, anatase and rutile. The gas was assumed to be ideal and the condensed species were introduced to the calculation as stoichiometrically invariant substances. The non-ideal properties of the slurry were thus neglected. The standard thermodynamic data for most of the compounds could be found in the databases and standard tables, for some like $TiO_2 \bullet nH_2O$ with n = 1,2 estimates derived earlier [7] were used. The heat transfer coefficients as well as the relevant radiation data were taken from litterature [8].

In the model, the drying and heating zones are assumed to be controlled by heat transfer and thermodynamics, while in the rutilisation zone reaction kinetics is combined with the thermochemical model. The salient time-dependent reaction is the formation of rutile $TiO_2(R)$ from anatase $TiO_2(A)$:

$$TiO_2(A) \rightarrow TiO_2(R) \qquad (4.1)$$

for which the extent of reaction can be written in terms of time t as follows [9, 10]:

$$\xi_R = 1 - \exp(-kt^n) \qquad (4.2)$$

where $k = A\exp(-E_a / RT)$ which is the temperature dependent Arrhenius reaction rate. The parameters A (the frequency factor) and E_a (the activation energy of the reaction (4.1)) are determined experimentally [8]. In the thermodynamic system, for setting correct heat and mass transfer balances during the rutilisation reaction, the rutile is used as a separate image component [11].

The counter-current streams of the gas and the slurry are both divided to volume elements which exchange heat and matter with each other and the surroundings. The streams encounter each other in a "zipper" iteration which converges according to the outlet and inlet temperatures which are known by process measurement. The overall heat balance is checked by including the propane burner in the multicomponent thermochemical model. In Fig. 5 the calculated temperature profiles of the kiln are shown. The wall temperatures are compared with measurement.

The static model brings about useful physico-chemical information of the normal operating data. Thus the stationary operation of the kiln can be simulated in varying process conditions. The first principles model as such is, however, tedious to apply to transient phenomena. This is mainly due to restrictions of computer time but also, to the neglect of axial gradients in the present model structure. The stationary information of process trends could yet be utilised to support the cohice of the variables in the dynamic process model which was directly based on process experience.

5 Dynamic simulation and control studies

The schematic diagram of the dynamic model is presented in Fig. 6. The model was developed as a “black-box” model. The content of the desired crystal form is considered the most important quality measurement of the process. The sampling interval of the process was initially two hours and the sample was taken manually. The transportation and handling of the sample form a significant delay in the control loop.

Manipulated variables m_1 and m_2 were considered possible alternatives for control. They can be controlled with controllers that are fast in relation to the dynamics of the calcination process itself. Therefore their measured value is approximated to follow their setpoints perfectly.

Process upsets are primarily caused by changing feed quality and quantity. The quantity of the feed can be measured on-line.

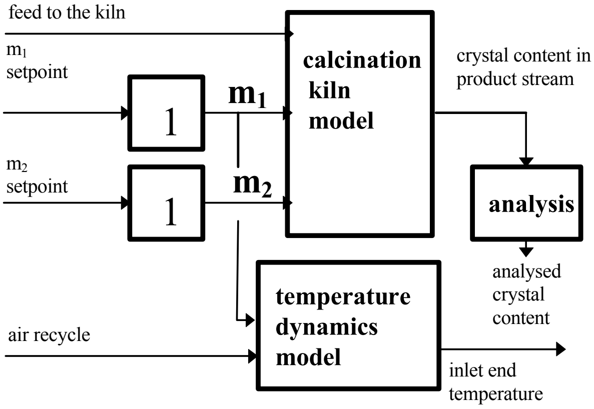

Fig. 6 The structure of the dynamical model

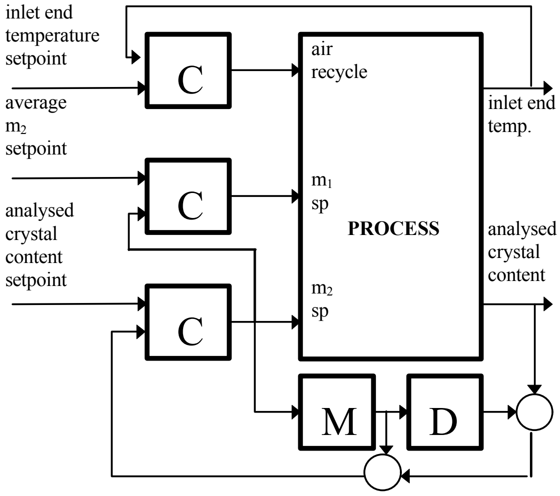

Fig. 7. A control strategy for the calcination kiln process. Controllers are marked with C. M is a simplified model. D is pure delay.

The control structure in Fig. 7 was presented. The crystal content of the product is primarily controlled by a fast acting manipulated variable m_2. Smith-predictor structure is used. The measurement is updated at discrete times.

The average of m_2 is kept at a desired level by manipulating m_1. This manipulation is slower than that of m_2. The original control was done by manipulating m_1.

In Fig. 8 the simulation model is used for the evaluation of the importance of the constant sampling interval and the improved representation of the samples that may be produced by using automatic sampling techniques. Slurry feed is increased 10 % at time 0. Moreover, white noise disturbance is presented during the whole time of simulation.

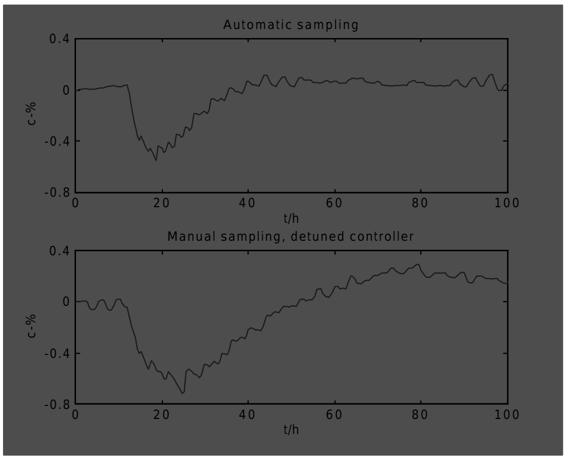

Fig. 8. Simulation results for the evaluation of sampling. First curve shows the control result with a constant sampling interval and improved representation, the second with the uncertainty caused by manual sampling.

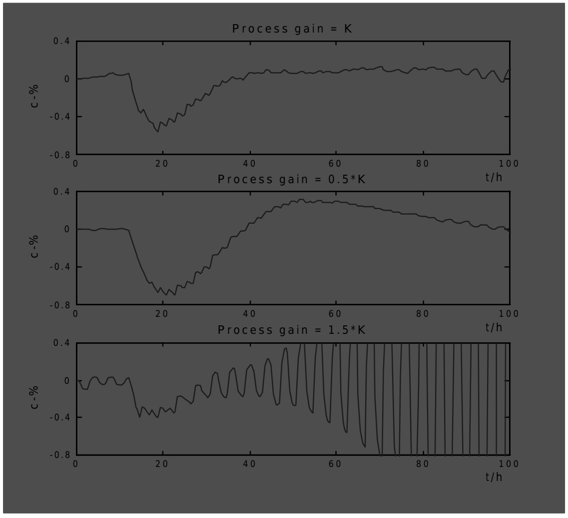

Fig. 9 Simulation results with constant tuning parameters and changing reaction kinetics of the

system .

In the first curve of Fig. 8 the system has been simulated with the automatic sampler that reduces the variability of the analysis results and makes the sampling interval constant. In the second curve the controller has been de-tuned to achieve stable operation.

Moreover, the predictability of the behaviour of the overall system depends highly on the reliability of the constant sampling period.

In Fig. 9 the effect of the changes in the reaction kinetics is evaluated by simulating the system with different process gains. This corresponds to the different pre-treatments of the slurry for different grades and the significant changes in the speed of the reaction in the kiln.

It may be assumed that operators who control the process manually tend to use similar control actions for different grades. This leads to sub-optimal behaviour of the system.

Static model of the process may be used to find different kinetic properties for the reaction of different grades. These properties may be introduced to the model incorporating structure of the control scheme fairly easily. Gain-scheduling techniques can be used.

6 Conclusion

In this paper the economic justification for the development of two simulation models for the same process has been presented. Modelling is proved to be a major source of improved process knowledge. The benefits may rise from different sources directly (on-line process control) or indirectly (improved insight).

Static and dynamic simulation models for a calcination kiln process are presented. These are used in the development of a control scheme for a process. This scheme may easily contain new information about the process that may be developed in the future.

The future work will include the use of these models for the development of improved measurements, control devices and algorithms for this process.

Acknowledgements

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