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Björn Kvarnström^a & Bjarne Bergquist^a

^a Quality Technology, Promote, Luleå University of Technology, SE-971 87, Sweden

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Improving traceability in continuous processes using flow simulations

Björn Kvarnström[†] and Bjarne Bergquist*

Quality Technology, Promote, Luleå University of Technology, SE-971 87, Sweden

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Traceability is normally difficult to achieve in continuous processes, since there are no natural batch structures. In this article, we demonstrate flow-based simulation using process data to improve traceability in a continuous pelletising process. Using the simulation model, the engineers could test the impacts of process disturbances, identify cause and effect relations and aid control in case of process disturbances. In a field trial where the chemistry of an additive was varied during production of a special product, the simulation forecasts predicted the level of the chemical content after the plant within the errors that the engineers found acceptable.

Keywords: continuous process; traceability; flow simulation; pelletising; modelling; residence time

1. Introduction

A high level of traceability is important to identify causes for process variation (Duffin 1995), it is beneficial for process control (Oakland 1995) and it is a requirement in ISO 9001-2008 (ISO 9001, 2008, 7.5.3). Traceability is usually comparatively uncomplicated for discontinuous production (discrete or batch production), since identification markers such as bar codes or serial numbers can be attached to the product or packaging. In contrast, descriptions of traceability systems for continuous production processes are scarce. However, traceability systems for such processes may be important, the food and pharmaceutical industries often use continuous processes and are required to maintain a high level of traceability; see Flapper *et al.* (2002). Continuous processes contain several characteristics complicating traceability that are not usually discussed in the literature. One example characteristic that is problematic is the continuous flow of material, as traceability solutions normally rely on the definition of a batch (Skoglund and Dejmek 2007). Furthermore, the products often undergo multiple changes of states (powders, solids, liquids, etc.) when processed, which also impedes traceability (Kvarnström and Oghazi 2008).

Huda and Chung (2002) suggest the use of simulation models to better understand the production process and to see the effect of different production scenarios in, for example, food manufacturing processes. We argue that simulation models may also be used to achieve traceability in other continuous

processes. However, simulation of continuous processes tend to focus on specific process sections and/or problems, see, for example, Finnie *et al.* (2005), Van Puyvelde (2006) and Bhaskar *et al.* (2007).

The traceability accuracy of any modelling approach of a continuous process will depend on how accurately the model can predict the product flow. Finely meshed computational fluid dynamic models or discrete element methods for granular material have been used to simulate small process sections with continuous flows, see Bhaskar *et al.* (2007) and Finnie *et al.* (2005). In practice, the complexities of these models often result in computational times that quickly become impractical, and reduced accuracy in favour of swiftness may be a better, or the only viable solution. One approach using rougher estimates to create liquid food traceability using virtual batch calculations for a dairy has been presented by Skoglund and Dejmek (2007).

The purpose of this article is to develop a process simulation approach, and to describe and apply a simulation model based on process data and flow estimations for a continuous process. We also aim to identify limitations of the modelling approach, some areas of use and discuss the possibilities for generalisation to other areas.

The article contains six sections in addition to the introduction. Section 2 describes different ideal flows and how the flow behaviour in a real system can be estimated. Section 3 presents the process and the production scenario for which the simulation model

*Corresponding author. Email: bjarne_b@ltu.se

[†]Present affiliation: GE Healthcare, Umeå, Sweden

was developed and tested. In Section 4, the simulation model development is described. The application of the simulation model and the result of the simulation are presented in Section 5. Finally, the article is concluded and discussed in Sections 6 and 7.

2. Process flows

Any real flow of liquids, powders, slurries or pulps has geometrically dependent flow velocities. The flow will range from the ideal states *perfectly mixed flow* to *plug flow*. The one extreme, the perfectly mixed flow, suggests that the matter (fluid, powder, etc.) entering a process section is immediately mixed with all matter that was in it. Hence, in this type of flow, each infinitesimal volume of the section's content has the same properties (chemistry, temperature, microstructure, particle size, etc.) at any given time. The assumption of a perfectly mixed flow is often used for continuous-stirred containers.

The other extreme, the plug flow, implies that the matter entering a process section will remain unmixed when passing through it. Hence, there is a fixed residence time for each infinitesimal volume of the flowing matter. The plug flow approximation is often used to model flow behaviour in tubular reactors.

For ideal flows, the mean residence time of infinitesimal volumes in the system would be equal to the system space time, τ , defined as

$$\tau \equiv \frac{V}{v_0}(s), \quad (1)$$

where V is the volume (m^3) of the system and $v_0(\text{m}^3/\text{s})$ is the volumetric flow rate through the system.

All real flows exhibit flow gradients and will therefore be mixed to some degree. This mixing is dynamic and progresses over time. Real flow systems also often include, for example, short-circuiting (bypassing) and stagnant regions (dead-zones) (Fogler 2005, p. 979). Nonetheless, most real flow systems could be approximated using ideal flow assumptions with addition of, for example, short-circuiting variables and stagnant region variables (Fogler 2005). The flow behaviour of real systems may be estimated by additions of tracers to the input flow and by repeated measures of the exhaust tracer concentration profile (Fogler 2005, *op. cit.*, p. 871).

3. The exemplified process

The exemplified process consists of two iron ore pelletising plants owned by the Swedish mining company LKAB. Normally, these plants together produce

900 metric tons product per day, an iron ore pellet (hereafter pellet). The plants are fed by two water/iron ore powder slurries originating from different sources with differing iron ore properties (Figure 1). The slurries are then mixed to ensure that both plants produce similar pellets. After the slurry mixing stage, the slurry is dewatered in the filter section, and the dewatered powder is then either temporarily stored or fed to a mixer where a binder is added. After the mixer, the powder flow is split into several streams and stored shortly before it is agglomerated and rolled into pellet granulates. During the rolling operation, the pellets are sieved, so that oversize pellets are crushed and returned to the mixing station. The granulate streams are then merged and sintered, which is the final treatment before distribution to the customer. The sintering furnace also contains an internal backflow, where 20% of the sintered pellets are fed back to the furnace entry and used as thermal protection for the equipment.

Important quality characteristics of the pellets are stable chemical and physical properties. However, the company sometimes needs to induce variability into the production process for product development purposes. This article describes a case where a special pellet with a different chemical composition was to be produced. The volume needed was larger than what was practical to produce in a laboratory, and the pellets had thus to be produced in the regular production process. However, the special pellets had to be separable from the regular product since these pellets did not meet the specifications of the regular product. Changes of chemical compositions of the product take considerable time and the shift would, consequently, interfere with regular production. Therefore, the production engineers wanted to decrease the product change window to minimise production losses. One of the difficulties involved in reducing the experimental product period was due to chemical analyses. These analyses were considered too slow for the production control needs, since it usually took hours to receive laboratory results. Therefore, another method to control the process had to be developed.

4. Development of the simulation model

After discussing the control problem with the authors of this article, the engineers decided to use a flow simulation approach aided by chemical analyses to plan for and monitor the product change. To be useful, the simulation model had to be fast and accurate enough to improve the engineers' own estimates of how fast the changes would reach and leave different process sections.

Figure 1. A flow sheet of the two pelletising plants at LKAB in Malmberget.

The first step to create the model was to estimate the process flow mechanisms and gather relevant process data. This information was obtained through interviews of process engineers and through studies of internal documents. Engineers from different process sections and departments were interviewed and were asked to describe the flow mechanisms that they thought governed product flow at different process sections. Each process section's residence time was then estimated through space time calculations using Equation (1). The estimations were based on the mean production flow, container volumes taken from blueprints, and from discussions with the engineers. Table 1 summarises the results of these primary studies.

The flow mechanisms in Table 1 were based on engineers' guesses, mostly without supporting data. Nevertheless, the collected information identified the slurry containers as the section affecting traceability the most, since these containers generate the longest residence times. However, the engineers had only vague ideas of the flow behaviour in the slurry containers.

A tracer experiment was therefore performed to identify a suitable flow characteristic which suggested

that the slurry container flow could be approximated as perfectly mixed. Another result was that the containers had a stagnant dead volume that did not take part of the mixing and thus reduced the mixed volume (Kvarnström 2008). The active volume share for the slurry containers were estimated to be 0.61 for plant 1 and 0.75 for plant 2 based on the experimental data.

A flow simulation model of the process was built after mapping the process flows and residence times in MATLAB[®] with the SIMULINK[®] toolbox. Table 2 presents the process variables used in the flow simulation model for the various process sections. A stepwise overview of how the model was created is given in Figure 2. The appendix describes how the two flow types were simulated.

A complication for the simulation was that the product undergoes a change of state, from slurry to powder in the simulated plant section. This was dealt with by simulating the flow of the powder constituent only. This was possible since the liquid part was not of interest and the liquid share at different stages was known and constant. Another complication was the insufficient knowledge of the flow mechanism in the

Table 1. Description of the process sections in the two pelletising plants.

Process section	Function	Space time (h)		Flow mechanism, as estimated by process engineers	Physical state for the product flow
		Plant 1	Plant 2		
Additive container	Store of additive	3.3	3.3	PMF with a 25% dead-zone	Slurry
Additive mixing container	Mix of additive with concentrate	0.02	0.02	PMF	Slurry
Slurry container	Buffer and mixer	7.05	6.85	Insufficient process knowledge	Slurry
Mixing container	Mixing of the two slurries	0.02	0.02	PMF	Slurry
Filters	Dewatering	0.06	0.03	PMF	Slurry
Iron powder storage	Buffer and mixer	0	1.5	Insufficient process knowledge	Powder
Mixer	Mix concentrate with binder	0.01	0.01	PMF	Powder
Bin	Buffer	0.7	1.2	PF	Powder
Balling equipments	Balling formation	0.1	0.1	PF followed by PMF	Powder
Sintering furnace	Sintering	0.5	0.5	PF with reflux	Powder

Note: PMF, perfectly mixed flow; PF, plug-flow.

iron powder storage bin. This complication was handled using two parallel simulations, differing only in which of the two ideal flow types was used for powder flow through this bin. The simulation results only differed marginally and a perfectly mixed flow was therefore assumed for the bin.

5. Production of the special product

The engineers wanted to know how to select production rates and buffer volumes to reduce the product change window before the special product was produced (hereafter, *the field trial*). The authors made initial simulations varying these parameters to see their effect on the production window, and to find means of minimising the time needed for the change. The simulation results of the progression of chemical compositions in the product for various process conditions were then discussed with the engineers. Such conditions could for instance be shifting buffer levels and production speeds. Based on the outcome of these simulations, the engineers discussed various control strategies, calculated the preliminary time for product removal, scheduled various resources and generated operator guidelines. An important guideline was to keep buffer levels low, just large enough not to risk material shortage to minimise the production of secondary product and change periods. This way, the chemistry would change more quickly due to a minimum amount of product mixing.

The authors made a new simulation at the start of the field trial, using actual levels and flows in the process for the simulation. This simulation was performed to assist detailed planning of the

product change, to foresee future events during the change, and to plan for preventive actions for unwanted events. Furthermore, the outcomes of various actions were simulated beforehand to aid decision-making.

At the beginning of the field trial, the production personnel discovered that a buffer was running low. The production rate would have to be reduced if the buffer would run out of material. One possible solution to avoid that problem was to pump slurry from another container, and with the model, the engineers could study the effect of the control action and decide whether it was suitable.

Laboratory results of the samples taken from the process were continuously used to calibrate and fine-tune the simulation results during the field trial to improve predictions of the change in chemical composition. The new data also made it possible to better estimate the dead volume in the various buffers and to adjust the model for improved estimates of the type of flow that the product had in different sections. However, these adjustments were small and the improvement of the simulation results was considered marginal by the engineers.

The simulation model was originally designed to simulate a process where the process variables were constant during the simulation period. However, the process variables varied during the field trial. The assumption that the variables were constant resulted in an unnecessary large simulation error. Therefore, the simulation model was modified to include logged process data in addition to the static data obtained during the start of the field trial. The model change improved the fit between the simulation output and the analysis data; see Figure 3. The changes between the initial simulation model and the final simulation model are highlighted in Table 2.

Table 2. The process variables used to model each process stage, what each variable was based on, and if the variable was varied or kept constant during the simulation.

Process stage	Process variable	Data collection ^a	Input ^b	
			Initial model	Final model
Additive container	Pulp density	Process data	Constant	Constant
	Weight per cent solid	Process data	Constant	Constant
	Buffer level	Process data	Constant	Varied
	Volume flow (in)	Process data	Constant	Varied
	Volume flow (out)	Process data	Constant	Varied
	Additive quota	Process data	Constant	Constant
	Active share	Estimated	Constant	Constant
	Maximum volume	Equipment data	Constant	Constant
Additive mixing container	Pulp density	Process data	Constant	Constant
	Weight per cent solid	Process data	Constant	Constant
	Volumetric flow (in and out)	Process data	Constant	Varied
	Volume	Equipment data	Constant	Constant
Slurry container	Pulp density	Process data	Constant	Constant
	Weight per cent solid	Process data	Constant	Constant
	Buffer level	Process data	Constant	Varied
	Volume flow (in)	Process data	Constant	Varied
	Volume flow (out)	Process data	Constant	Varied
	Active share	Estimated	Constant	Constant
	Maximum volume	Equipment data	Constant	Constant
Slurry divider	Proportion slurry to plant 1 from slurry container plant 1	Process data	Constant	Constant
	Proportion slurry to plant 1 from slurry container plant 2	Process data	Constant	Constant
Mixing container	Pulp density	Process data	Constant	Constant
	Weight per cent solid	Process data	Constant	Constant
	Volumetric flow (in and out)	Process data	Constant	Varied
	Volume	Equipment data	Constant	Constant
Filters	Pulp density	Process data	Constant	Constant
	Weight per cent solid	Process data	Constant	Constant
	Volumetric flow (in and out)	Process data	Constant	Varied
	Volume	Equipment data	Constant	Constant
	Numbers of filters in use	Process data	Constant	Constant
Iron powder storage	Buffer level	Process data	Constant	Varied
	Volume flow (in)	Process data	Constant	Varied
	Volume flow (out)	Process data	Constant	Varied
	Active share	Estimated data	Constant	Constant
	Maximum volume	Equipment data	Constant	Constant
Mixer	Volumetric flow (in and out)	Process data	Constant	Varied
	Volume	Equipment data	Constant	Constant
Bins and Balling equipment	Buffer level	Process data	Constant	Constant
	Volumetric flow (in and out)	Process data	Constant	Varied
	Volume bin	Equipment data	Constant	Constant
	Number of bins in use	Process data	Constant	Varied
	Volume of the balling equipment ^c	Estimated data	Constant	Constant
Sintering furnace	Time in furnace	Equipment data	Constant	Constant
	Return flow	Equipment data	Constant	Constant

Notes: ^aProcess data is data collected by the ordinary process system. The process data may vary over time and is controlled by the engineers. Product data is data decided during the manufacturing of the equipment and constant over time. Estimated data is data that is/cannot be measured or controlled during normal operations. The estimated data is therefore based on previous experiences or on estimations from process engineers.

^bThe models used two types of input, either a constant value or a times series of data from the process. In this case the constant values were decided beforehand or at the start of the experiment.

^cThe balling equipment was modelled as a plug flow followed by a perfectly mixed flow.

Figure 2. The stepwise approach used to create a simulation model based on simple flow assumptions.

Figure 3. Comparison of the fit between the predicted level of chemical content in pellets after the sintering furnace in Plant 2 for analysis data and simulation output for the first simulation model and the final simulation model. The final simulation model was fitted to the actual buffer levels and flows in various process sections at different times, whereas the first simulation model was based on static estimations of buffer levels and flows using initial measurements. The units and exact measurements on the ordinate are withheld due to proprietary reasons.

6. Discussion of the modelling results

According to the LKAB engineers, the field trial was successful and the simulation model had performed better than expected and provided important input. However, the process contained sections where the engineers often had to adjust flows or buffer volumes during production or during experiments. Therefore, the engineers saw the ability to link the model to current volume measurements as an important improvement.

Nevertheless, even if the engineers stated that the initial model had produced valuable results before and during the experiment, the first simulation results that were not based on logged data predicted a faster change of the chemical content than experienced. The major reasons for this difference were that the initial model was based on larger process flows and smaller buffer volumes than what were seen during the field trial. This sensitivity versus incorrect flow and buffer volume assumption was known before the experiment and several simulations with differing flow and buffer volumes were therefore made and the results discussed with the engineers. The deviation between the predicted and the actual chemical change stresses the importance of correct assumptions, and the possibility to vary the flow in the simulation model over time was another major improvement. Additional improvements would probably require better flow estimations and new tracer experiments.

Mixing is one characteristic that differentiates continuous processes from discrete processes. Two effects of mixing were seen in the simulations, disturbances were smoothened and the impact of changes delayed. Mixing reduces the amplitudes of disturbances downstream, but the effect is also prolonged. In addition, the degree of mixing depends on the process and how it is operated during the disturbance (volume of containers and speed of mixers are examples of process settings that will influence system response). The maximum tolerable duration and amplitude of a disturbance will vary depending on the sensitivity of downstream operations. The process model could be used to aid the design of the process, given how large variation that is acceptable.

7. Main conclusions and findings

In this article, we have presented a stepwise approach for creating a simulation model of a continuous process based on ideal flow assumptions that may visualise and help to control and reduce the impacts of process disturbances. In the general case, such simulations may aid finding root cases, find control actions

to reduce effects of disturbances and to help redesign production processes so that intolerable disturbances does not reach the customers. The case study shows how process data coupled with simulation may increase the traceability of the product within a continuous process where normal laboratory analysis of samples is too slow.

We argue that process simulation could be used in many cases where normal sampling is too infrequent or laboratory analysis of samples is too slow for control purposes, but agree with Cox *et al.* (2006) that simulation speed is a key to efficient use of simulations. Cox *et al.* (2006) state that simulations should be at least about 50 times faster than real time to be useful. Although the true number must be application dependent, it may be noted that the presented simulation model speed was 500 times faster than real time on a regular PC and that the simulation times made testing different control strategies fast and easy.

The impact of a process change upstream in the studied process was delayed, and an upstream disturbance would not affect product properties for several hours. We believe that such dynamic characteristics are common in many continuous processes and the effects of operator's actions in continuous processes are therefore often invisible during their working shift. Such delays may hinder operator learning. The simulation model we used provided a satisfactorily accurate prediction of the process response to a given disturbance. Therefore, the model could be and was used for predicting effects of corrective actions. Hence, the model may facilitate operator learning as the model can simulate the result of a process change with sufficient accuracy. The simulations offered predictions of the amplitude, longevity, and whereabouts of process shifts, other than providing understanding about the process lag.

If the process is to produce different products, such as in the exemplified case, there is a need to estimate the location of the shift, possibly at several positions and times. A use of the simulation model could be to estimate when a product will enter various process sections.

Another application would be for process control purposes. Control actions performed in a process are usually based on various measurements. However, some properties may only be measured through laboratory analysis, which is usually too slow for most control purposes. From our demonstration, we conclude that process simulations could provide decision support in such cases as the simulation can predict the development of the property of interest.

As with any model, incorrect assumptions will affect the correctness in the output. For the studied process, the simulation model was based on existing process knowledge and calibrated using a small experiment, and the simulation results did, according to the engineers, correspond well with the measurements taken during the change. A simple model based on existing process knowledge may therefore be sufficient for continuous processes like the one studied here.

Process analysis using time series methods may be another easily obtainable option to create traceability models for continuous processes. Time series analysis may be used to link disturbances on inputs to effects on outputs, whereby a traceability model could be constructed; see Vanhatalo *et al.* (2011). Such an empirically based model would be very fast, but has the disadvantage of being a static black box. Trusting results of a black box model is risky if the process has undergone changes that were not part of the original experiment. Nonetheless, such models could be easily set up and could prove useful for processes where different operating modes and equipment changes are rare.

Other means of creating traceability have been suggested for continuous processes for granular media, e.g. radio frequency identification (RFID) markers in a pellets distribution chain (Kvarnström and Vanhatalo 2010), but more work is needed in that field.

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Notes on contributors

Björn Kvarnström is Product Quality Specialist at GE Healthcare. He holds a PhD in Quality Technology from Luleå University of Technology (LTU). He holds an MSc degree in Industrial and Management Engineering from LTU and a Licentiate degree of Engineering in the subject of Quality Technology and Management from LTU. His current research is focused on methods to improve traceability in continuous processes. He is a member of ENBIS.

Björn Kvarnström is Product Quality Specialist at GE Healthcare. He holds a PhD in Quality Technology from Luleå University of Technology (LTU). He holds an MSc degree in Industrial and Management Engineering from LTU and a Licentiate degree of Engineering in the subject of Quality Technology

Bjarne Bergquist is a Professor and Chair of Quality Technology and Management at Luleå University of Technology. He holds a Master's degree in Mechanical Engineering from Luleå University of Technology and a PhD in Materials Science from Linköping University, Sweden. His main research interest is focused on

process control and experimental design, especially for continuous process applications. He is a member of ENBIS and ASQ.

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Appendix

The simulation model contains 14 different steps, see Figure A1. All the process steps were designed individually in SIMULINK® and then connected in process order. In the simulation model the two plants were kept apart, except for the slurry divider. Each process section was either constructed as a perfectly mixed flow or a plug-flow in accordance with the identified flow in Table 1.

The model structure of a section classified as a perfectly mixed flow is demonstrated in Figure A2 and the structure of a section classified as a plug-flow is demonstrated in Figure A3. In the modelled section, the inflow volume, the concentration in the inflow for the substance of interest, the outflow volume and the active volume of the section are

Figure A1. The different sections included in the simulation model in flow order and the assumed flow for the different sections.

known. The purpose of the model was to predict the chemical concentration of the current and future exhaust flows of the section.

The first step is calculating the amount of substance entering the perfectly mixed system. This is done by multiplying the inflow volume by the concentration of the substance in the inflow. The incoming amount is then added to what is already present in the system (remaining amount in Figure A2). The substance leaving the section is calculated through multiplying the entire amount of the substance in the section by the volumetric ratio leaving the section. Finally, the remaining amount in the section is calculated by subtracting the exiting amount from the entire amount in

the section. The exiting amount is then used in the next simulation step.

As with the perfectly mixed system, the first step to predict the chemical concentration in a plug-flow system (e.g. a container) is to calculate the amount of the substance that is entering it. Again, the amount entering a system is given by the inflow volume multiplied by the concentration of the inflowing substance. For plug-flow systems, the concentration of the substance flowing out of the system is identical to the concentration of the substance entering it, but with a delay given by dividing the system volume by the outflow. The exit concentration and flow is then used for the simulation of the following process step.

Figure A2. A graphical display of how a perfectly mixed section is designed in the simulation model. The grey boxes are mathematical operations while the white boxes describe the variable resulting from an operation.

Figure A3. A graphical display of how a plug-flow section is designed in the simulation model. The grey boxes are mathematical operations while the white boxes describe the variable resulting from an operation.