STATISTICAL PROCESS CONTROL MODELS IN AGRO-CHAINS

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Introduction: Statistical Process Control

Consumer expectations on quality of food products are very high and tend to increase as well as diversify to include flexible and fast delivery, health, safety and minimal environmental impact. Assurance to conform or even exceed these expectations can no longer come from mass inspection, but has to be founded on intelligent process control, process and product design and continuous improvement. Statistical Process Control (SPC) provides the sound basis for this. Although SPC used to be strongly associated with the statistical tools applied, it is now regarded in general as an indispensable approach to managing processes (Deming (1986), Snee (1990), Joiner (1994), Hare et al. (1995), Hoerl (1995), Does et al. (1997), Roes and Dorr (1997) and Roes (1997)). In the broader context this approach is based upon the principles that:

- all work is a series of interconnected processes;
- all processes vary;
- sources of variation can roughly be distinguished as arising from common causes (inherent to the process as designed) and special causes;
- understanding the origin of each of these sources of variation is the key to reduction of variation;
- reduction of variation is the key to quality improvement, productivity and profitability.

Statistical methods such as control charts, experimental design, data analysis are applied to uncover causes of variation and thus control and improve the processes. SPC can be implemented on the shop floor by cross-disciplinary teams, called Process Action Teams (PATs). In production processes such teams consist of operators, foremen, process-engineers, maintenance-engineers and other technical personnel involved with the process, and a statistician. A PAT implements SPC for a specific process following a stepwise approach, based on the Plan-Do-Check-Act cycle. This forms a close link between statistical thinking and the scientific method. The main steps are:

I. Definition of the process to be dealt with
II. Diagnosis of the process
III. Actions and measurements
IV. Design of feedback control loop
V. Implementation and further improvement (back to I)

The result of the phases I through V is usually twofold. The main purpose is to install a control loop with control charts and accompanying out of control action plan (Figure 1). In this control loop, deviations from the normal performance of the process are detected by means of control charts. Subsequently, the shop floor operators follow the out of control action plan to identify and remove the cause as quickly as possible. Concurrently with establishing this control loop, opportunities for improvement arise during process diagnosis and appropriate action is taken or is planned to be taken once control is established.

The process diagnosis is a crucial step and includes describing processes using flow-charts and performing a risk analysis based on the Failure Mode and Effect Analysis (FMEA) technique (see Stamatis, 1995). Possible causes and effects critical quality characteristics

are generated, and rated based on severity of the effect, frequency of the cause and effectiveness of installed inspections. If necessary, these assessments can be substantiated by performing designed experiments. Thus, this provides the basis for improvements and identification of the critical product and process parameters to measure and control.

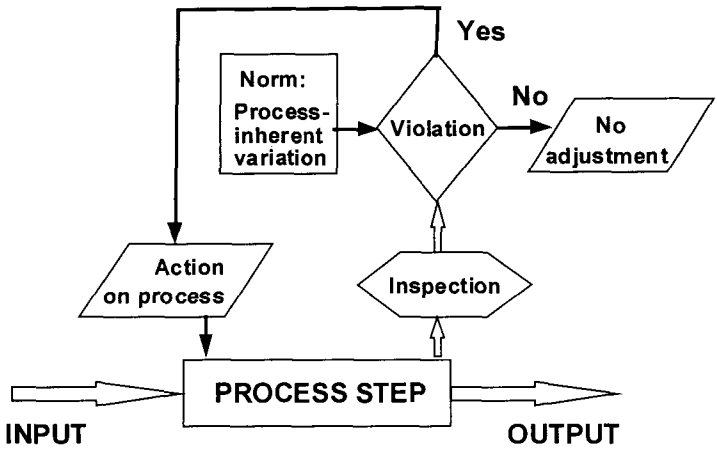

Figure 1 SPC control loop.

SPC and SPC methods are implemented in several major (food) industries in the Netherlands (Does, Roes and Trip, 1996), although not often with the above presented strong involvement of the shop floor. Good examples include (parts of) Unilever and Sara Lee/DE. There still are major gains in quality and costs to be made with more rigorous implementation. This holds with respect to the involvement of the shop floor workers in process control implementation as well as to the statistical methods applied. The latter traditionally start form rather uncomplicated process models, which basically assume that process quality characteristics vary randomly around a constant mean level. Extensions that have been applied involve incorporating variance components (e.g., Roes and Does, 1995) and applying time-series modelling (see Box and Kramer (1992) and the recent discussion by Montgomery and Woodall (1997)). Strikingly absent in most published applications are monitoring and control schemes based on physical or chemical models underlying process behaviour. These seem particularly relevant for processes in agro-chains. In this paper we will briefly review current practices with respect to control charts for SPC and underlying models, focusing on the basic models and incorporating additional variance components. This will be illustrated with an example from the production of butter, without elaborating on the statistical theory involved. Next we will discuss application of an approximate model incorporating production settings for process yield in a refinery. This is based on a real (agro-chain) example, which cannot be revealed in full detail due to confidentiality agreements. It will be shown how proper monitoring schemes can be derived from such a model and to what extent they are superior to more basic models. Implications will be discussed as well as the direction of further modelling to be developed.

Basic models for control charts

Originated by Shewhart in 1924 (see Shewhart (1931)), the effectiveness of control charts is due in part to their simplicity. They consist of a graph with time on the horizontal axis and a control characteristic on the vertical axis. Control limits drawn provide easy checks on the stability of the process: no special causes present. The charts are usually

constructed using 20 to 30 initial samples of about 5 units from the process at hand. In general, these samples are supposed to arise from pure random sampling, when chosen 'rationally': rational subgroups (see Nelson (1988)). Ideally, such a subgroup is chosen to be a sample in which all items are produced under sufficiently similar conditions. This ensures that only random effects are responsible for the observed variation. The variation within a sample is supposed to represent all variation attributable to common causes. It then follows that the within-subgroup variation can be used to determine the variability of the subgroup quality characteristics, such as the sample mean or range. Control limits are calculated using a measure of within-subgroup variation. Hence, the basic model in case the process is in control for this standard situation is as follows:

$$Xtj = \mu + Etj, \qquad (1)$$

where X_{tj} are the measurements of the quality characteristic, with t indexing time, and j=1,..,n indexing the unit within the sample taken at time t. E_{tj} models the random variation within a sample. It is usually assumed that the E_{tj} are all mutually stochastically independent variables, normally distributed with means 0 and variance σ_e^2, respectively. Limits for the control charts on the mean level per sample are set at: Central Line (CL)= μ, Upper Control Limit (UCL) = $\mu + 3\sigma_e/\sqrt{n}$ and Lower Control Limit (LCL) = $\mu - 3\sigma_e/\sqrt{n}$. See for more extensive discussion on setting limits in case parameters have to be estimated Does and Schriever (1992) and Roes et al. (1993).

Example

In control of butter quality it is in the interest of both producer and consumer to control the water content of the final product (in terms of relative weight percent) within tight limits (van der Voet, 1996). European Union regulations require that this water content should be demonstrably below 16%. In this example we examine data from the process form a large dairy producer, taken during 1 month. The data consist of one sample per pallet on 16 days. The number of pallets sampled varies between days, depending on production. Based on the basic model (1), a control chart for each individual measurement was drawn (i.e., n=1 in the above model).

Limits were based on the first 76 samples (3 days of production). The standard deviation σ_e was estimated by the mean moving range (see Roes et. al. (1993)).

Figure 2 clearly shows several out of control conditions beyond the first period (after 76 pallets). These are around the 100th pallet, the 155th and between the 200th and 250th. It is also obvious, that these out of control conditions occur in clusters, suggesting either correlated observations over time, or that the process control and adjustment frequency is not per pallet but more likely per day.

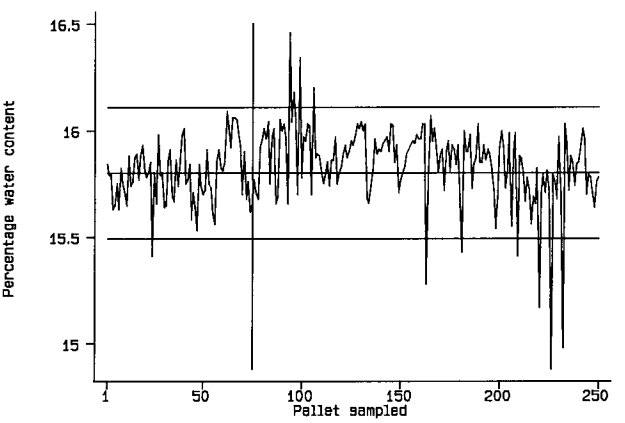

Figure 2 Control chart for individual measurements of % water content in butter.

Correlation between consecutive observations (autocorrelation) suggests time-series modelling. This has been developed in conjunction with SPC in recent years (see e.g.,

Box and Kramer (1992), Box and Luceño (1997) and Montgomery and Woodall(1997)). As Box and Luceño (1997) show, an Exponentially Weighted Moving Average (EWMA) presents an optimal monitoring and adjustment instrument in case of a basic time series model.

This model applies to the butter example as follows: from (1) $X_t = \mu + E_t$ where X_t are the water content measurements and E_t models random disturbances. In (1) these were assumed independent. A basic time-series model assumes:

$$E_t - E_{t-1} = A_t - \theta_0 A_{t-1} \quad (2)$$

where A_t is a series of statistically independent errors, with mean 0 and variance σ_a^2. This model can be interpreted as follows: the deviation from target at time t equals the deviation form target at the previous observation plus a random shock A_t and plus a (proper) fraction θ_0 of the previous random shock. For the EWMA the following quantities are charted:

$$Z_t = \lambda (X_t - m) + (1- \lambda) Z_{t-1} \text{ for } t=1,2,3,..... \quad (3)$$

with $Z_0 = 0$. The X_t are centred with a mean level m, estimated on the basis of an initial sample, which in this example consists of the first 76 observations.
Limits can be set at +/- K $\sigma_e \sqrt{\{\lambda(2- \lambda)\}}$, where λ can be determined as estimate of $(1- \theta_0)$ in model (3) or according to certain optimality criteria of the EWMA chart. As stated in Quesenberry (1995), λ=0.25 and K=2.90 represent an acceptable balance between the in-control and out-of-control performance of the procedure. The EWMA chart based on these choices and the standard deviation and mean estimated from the first three days of production (76 samples) is shown in Figure 3.
The EWMA more powerfully detects out of control conditions, demonstrating the same clustering of incidents. As such, it is an improvement on the previous model and accompanying charts. The time series of measurements does display auto-correlation (ranging from 0.37 between consecutive observations to practically zero between observations more than 5 apart). The fact that the nature and cause of the auto-correlation is not revealed, remains unsatisfactory.

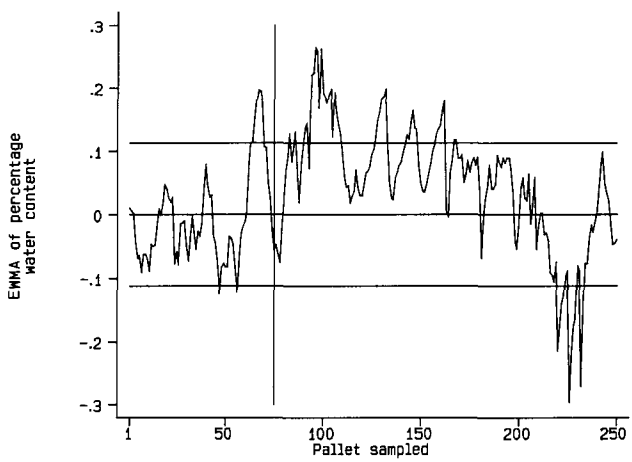

Figure 3 EWMA chart of water content in butter data.

Application of variance components models

One phenomenon that may give rise to correlated observations, is the presence of several (nested) components of variation actually present in the process. An alternative approach to just modelling the autocorrelation, is to identify and quantify the components of variation and use them as basis on which a useful distinction between special and common causes can be made. Control charts should then be designed to control all relevant components of the common cause system, on the basis of 'rational sampling': sampling plans that are

purposely not random and aim to describe the important variance components (Palm (1992)). Examples are: sampling from several (fixed) positions on a mould and several (fixed) leads from the same equipment. A somewhat different example is sampling from (chemical) batches, where there may be extra between-batch variation due to the fact that raw materials, set-up and adjustments usually vary between batches. The sampled subgroups for these processes will show systematic within-subgroup variation and occasionally additional between-subgroup variation. The methodology to determine control limits for appropriate subgroup statistics can be more involved, although plausible simple alternatives have been recommended. Roes and Does (1995) describe a method applicable to cases with both fixed differences within a sample (position on a silicon wafer for integrated circuit manufacturing), and extra between-batch variation.

Example (continued)

To elaborate on the general ideas, we continue the example of dairy butter. We observed out of control conditions occurring in clusters. Moreover, the process is such that adjustments are not made continuously but periodically. Thus, it seemed more appropriate to evaluate the process in 'batches' and consider each set of 6 pallets as a subgroup and the individual pallets as samples within this subgroup (recall the fact that the auto-correlation is practically 0 for measurements more than 6 apart). The model than becomes:

$$Xtj = m + Bt + Etj, \qquad (4)$$

where X_{tj} are the measurements of the percentage water content, with t indexing the subgroup (batch), and j=1,..,n indexing the pallet within the subgroup taken at time t. E_{tj} models the random variation within the sample (batch) of n pallets. It is assumed that the E_{tj} are all mutually stochastically independent variables, normally distributed with means 0 and variance σ_e^2, respectively. B_t models the random between batch effects; the B_t are mutually independent, normally distributed with means 0 and variance σ_b^2. As a consequence of this model, X_{tj} 's from different batches are stochastically independent. X_{tj} 's from the same batch, however, are correlated with correlation coefficient $\sqrt{\{\sigma_b^2/(\sigma_b^2 + \sigma_e^2)\}}$.
Control charts are now developed for the mean level per batch as well as the variance within a batch. Limits for the control charts on the mean level per sample are set at: Central Line (CL)= μ, Upper Control Limit (UCL) = $\mu + 3\sqrt{\{\sigma_b^2 + \sigma_e^2/\sqrt{n}\}}$ and Lower Control Limit (LCL) = $\mu - 3\sqrt{\{\sigma_b^2 + \sigma_e^2/\sqrt{n}\}}$ (Figure 4). See for more extensive discussion on setting limits in case parameters have to be estimated Does and Schriever (1992) and Roes en Does (1995).
Limits for the estimated standard deviation within a batch, s_e^2, are based on the fact that under model (4) s_e^2 is distributed as $\sigma_e^2/(n-1)$ times a chi-squared distribution with n-1 degrees of freedom (denoted by χ^2_{n-1}). Hence, the lower and upper limits are set at $s_e\sqrt{\{\chi^2_{0.01,n-1}/(n-1)\}}$ and $s_e\sqrt{\{\chi^2_{0.99,n-1}/(n-1)\}}$, respectively, where $\chi^2_{\alpha,n-1}$ denotes the α-th percentile of the cumulative χ^2_{n-1} distribution.
In the example at hand the first three days of production yielded: $s_e = 0.118$ %, $s_b = 0.064$ and hence the correlation coefficient within a batch is 0.265. Thus, it is clear that there is extra between batch variation (long term) in addition to the short term variation between pallets. The corresponding control chart is shown in Figure 5.
The charts based on model (4) show a more concise picture of the process compared to the ones displayed previously. Figure 4 indicates a jump in mean level of percent water content at the 15th batch, which retrospectively probably started at batch 13. This jump persists until beyond the 30th batch. The control chart for the within batch standard deviation indicates batch 14 with excessive variation between pallets. Moreover, the within batch standard deviation increases toward the end, leading to four out of control conditions.

The key issue is the fact that these charts lead to a more directed search for causes. The persisting rise in mean level indicates a lasting change in settings, process conditions or raw materials. The increased standard deviations relate to operating conditions changing at short notice. Probably operator influence or shop floor incidents were involved here.

In Roes and Does (1995) and Does, Roes and Trip (1995) the general methodology underlying this type of charts was developed and illustrated with several examples. These also illustrated the effectiveness of uncovering causes based on the charts signals. Their charts also included fixed effects between samples, which can be monitored with well-chosen differences within the samples. These are determined based on the model applied and the physical and chemical nature of the process at hand. This type of control charts has been successfully applied in numerous processes and industries. Building upon these general variance components models, a natural refinement will include models relating quality characteristics directly to process settings and conditions.

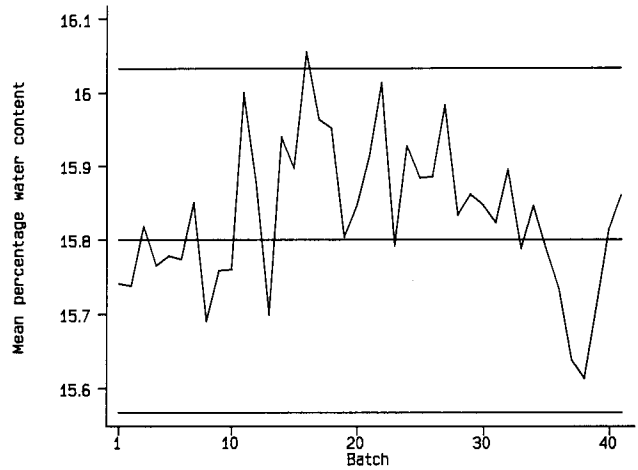

Figure 4 Control chart of mean water content in butter data. Based on nested variance components.

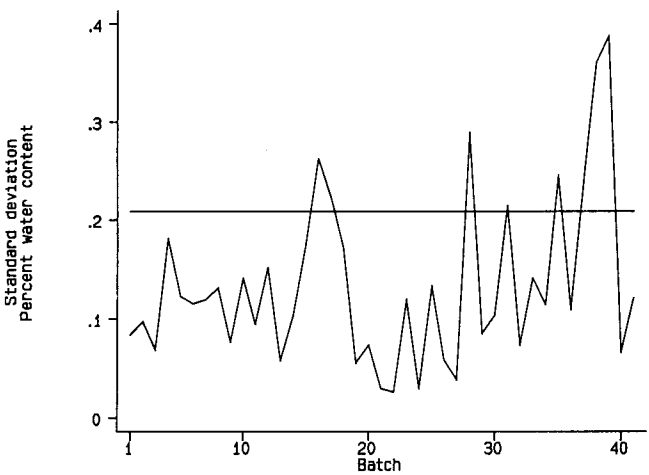

Figure 5 Control chart of within-batch standard deviation of water content in butter data.

Modelling dependence on influence factors

In the previous section SPC models did not include any factors or process settings directly influencing the quality characteristic under consideration. These may very well be known in practice and may also be known to vary during production. Factors and settings could include temperature, pressure or flow of equipment used as well as concentration of chemicals applied or present in the raw material. If the quality characteristic can be modelled as function of these factors and settings, this may improve the efficiency of the SPC control loop in several ways:

- the factors and settings can possibly be controlled tightly, thus eliminating sources of

variation;

- if factors and settings vary, their actual value may be measured precisely and control can be aimed at monitoring the difference between the quality characteristic as measured and as predicted by the model; this will increase the power of detecting special causes.

The model applied can be derived from chemical and physical models as well as through experimentation and empirical model building (Box and Draper (1987)).
To illustrate the general principles, an example derived from a large food industry is presented. Due to confidentiality agreements, details of the process and actual outcomes cannot be presented.

Example

In a chemical process to purify raw materials to be used in food applications, final yield is of major importance. From an initial large amount of factors and settings, four production settings and two raw material characteristics were shown to influence yield. The production settings involved concentration of two chemicals A and B, flow (F) and pressure (P). The raw material characteristics involved concentrations of chemical substances to be removed (C and D). Response surface experiments were run to determine a second degree polynomial approximating yield as function of these six factors (Box and Draper (1987), Box, Hunter and Hunter (1978)). This empirical road was chosen, since no valid theoretical models predicting yield as function of these factors could be posed. The experiments resulted in the following model for the yield (as measured in averages over 15 minutes, from continuous measurements):

$$\begin{aligned}\text{Yield}(\%) = \; & C_0 \\ & - 2.0(C - 4.3) - 13.0(D - 0.23) \\ & - 0.18A + 0.16B + 0.05B^2 - 0.12F - 0.15P + 0.07AF + 0.08FP \\ & + E \end{aligned} \qquad (5)$$

In (5), C_0 is the standard yield (93.2% in this case). The second line corresponds to raw material characteristics, the third to process settings and finally random variation (E) is present. A, B, P and F are coded between (-2,2) as standardised deviations from their nominal setting. (C - 4.3) and (D - 0.23) represent true deviations from their average values. E is considered to be normally distributed with mean 0 and standard deviation 0.12%, as estimated from the experiments.

Model (5) can be used to optimise the process; in this paper we will focus on control. To illustrate the advantage of the model, two possible control chart options are presented:

1. Directly charting the yield over time.
2. Estimating the yield using model (5) and the true (measured) values of A, B, P, F and C and D. Subsequently, the residuals: residual = (yield - estimated yield) are monitored with a control chart.

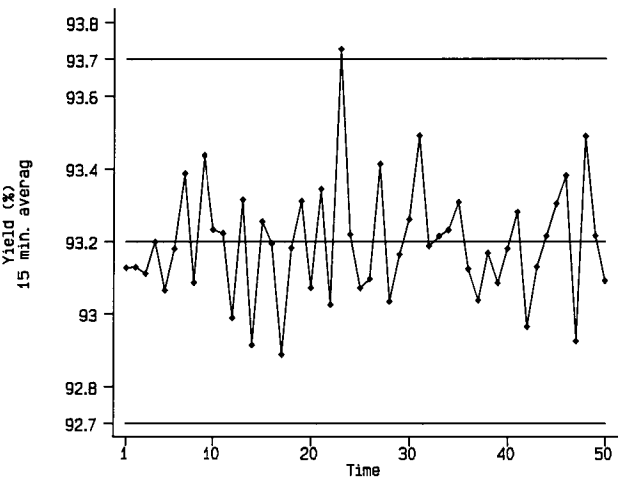

Figure 6 Control chart for process yield.

In this comparison it is assumed that the process factors in fact will show small variations over time, despite the fact that their settings may be fixed. This corresponds to the actual situation in many processes.
Figure 6 shows the control chart for the yield directly, based on simulated data. Apart form one out of control signal, no specific trends or shifts are visible. As these are simulated data, it is known that the one out of control signal is in fact false alarm.
The control chart for the residuals (yield - estimated yield) in Figure 7 does show up a clear feature: from the twenty-fifth observation onwards, the residuals are shifted upwards. The fact that 11 consecutive points are above the central line strongly indicates this (Nelson (1984)). Hence, the actual process yield is demonstrably larger than predicted with the current model. This means that a factor is at work, which may very well help to improve the process. From directly monitoring the yield, this would have gone unnoticed.

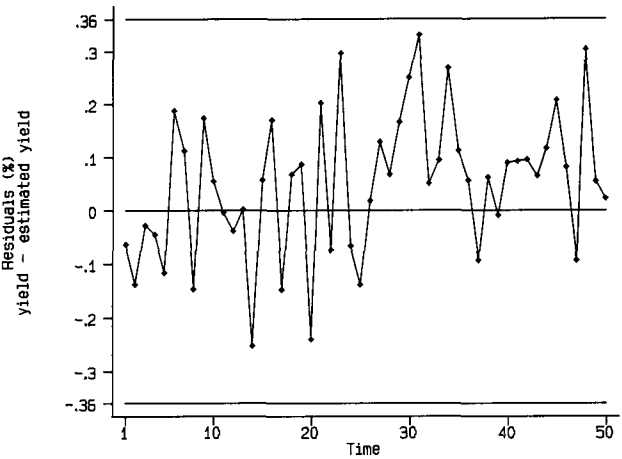

Figure 7 Control chart for residuals: process yield - estimated process yield.

In the actual process studied, such a factor is most likely related to characteristics of the raw material. This fact was used in the simulations, which mimicked a change in raw material at the 26th observation having a different effect as modelled. In practice, model (5) can also be used and extended to fine tune the process as quickly as possible to such changes in batches raw material.

Summary and conclusion

In this paper Statistical Process Control was briefly introduced, emphasising the importance of proper implementation in addition to statistical proficiency. A review of basic models applied in Statistical Process Control was given, illustrated by an example. Important extensions for many real life applications include modelling of variance components and modelling dependence on known influence factors. In both cases it was shown here, as well as in previous papers, that these models lead to more efficient detection of out of control conditions and more directed search for special causes. Specifically the methodology that includes modelling influence factors is new and under development. It is expected to be particularly beneficial to processes in agro-food production.

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