

RESEARCH ARTICLE

On- and Offline Detection of Structural Breaks in Thermal Spraying Processes

Matthias Borowski^{a*}, Nikolaus Rudak^b, Birger Hussong^c, Dominik Wied^b, Sonja Kuhnt^d
and Wolfgang Tillmann^c

^a*Institute of Biostatistics and Clinical Research, University of Münster, 48149 Münster, Germany;*

^b*Faculty of Statistics, TU Dortmund University, 44221 Dortmund, Germany;*

^c*Faculty of Mechanical Engineering, TU Dortmund University, 44221 Dortmund, Germany;*

^d*Dortmund University of Applied Sciences and Arts, 44227 Dortmund, Germany*

(Received 00 Month 200x; in final form 00 Month 200x)

We investigate and develop methods for structural break detection, considering time series from thermal spraying process monitoring. Since engineers induce technical malfunctions during the processes, the time series exhibit structural breaks at known time points, giving us valuable information to conduct the investigations.

First, we consider a recently developed robust *online* (also *real-time*) filtering (i.e. smoothing) procedure that comprises a test for local linearity. This test rejects when jumps and trend changes are present, so that it can also be useful to detect such structural breaks online. Second, based on the filtering procedure we develop a robust method for the online detection of ongoing trends. We investigate these two methods as to the online detection of structural breaks by simulations and applications to the time series from the manipulated spraying processes. Third, we consider a recently developed fluctuation test for constant variances that can be applied *offline*, i.e. after the whole time series has been observed, to control the spraying results. Since this test is not reliable when jumps are present in the time series, we suggest data transformation based on filtering and demonstrate that this transformation makes the test applicable.

Keywords: time series; jumps; trends; variance changes; Repeated Median regression; thermal spraying processes

1. Introduction

Industrial production processes are often supervised by the ongoing measurement of several variables. For example, the quality of thermally sprayed coatings can be controlled by monitoring the particle properties of the spray jet. Technical malfunctions typically lead to structural breaks like jumps and trend changes in the time series. They can also involve sudden or gradual changes in the variance of the time series. If such structural breaks can be detected *online*, i.e. in real time, the engineer can react so that production failures can be avoided. Furthermore, it is reasonable to assess the quality of the coating result *offline*, i.e. after the spraying process has finished, by watching for structural changes in the observed time series of the particle properties.

*Corresponding author. Email: matthias.borowski@ukmuenster.de

Reviews on mainstream methods for process surveillance and detection of structural breaks can be found in [2, 16], for instance. Recent articles in the Journal of Applied Statistics related to this topic are given by [3, 6, 10, 13, 14].

Scientists in engineering, mathematics and statistics of the Collaborative Research Center 823 of the Deutsche Forschungsgemeinschaft develop and investigate procedures for the on- and offline analysis of dynamic processes. In this study, the spraying processes are manipulated by the engineers to imitate critical technical failures. Hence, the time series of the particle properties exhibit structural breaks at known time points, giving us valuable information to assess the performance of detection procedures. We aim at three goals in this paper:

First, we consider the recently developed *Slope Comparing Adaptive Repeated Median* (SCARM) [5], a procedure for online filtering (i.e. smoothing) based on robust *Repeated Median* (RM) [18] regression in a moving window sample. The SCARM adapts the width of the time window to the current data situation at each time point by means of a test for local linearity. We assess the performance of this test as to the online-detection of jumps and trend changes by means of simulations and applications to the time series from the manipulated spraying processes.

Second, we propose a new robust procedure for the online-detection of ongoing trends, which is based on the SCARM filter. The performance of the trend-detection procedure is investigated by means of simulations and applications to the given time series.

Third, we consider a recently developed fluctuation test for the offline-detection of changes in the variance of time series [22]. This test assumes mean-stationarity of the process, which is not given for the considered spraying processes. Therefore, we propose data transformation based on robust RM regression to obtain mean-stationary time series that still exhibit the variance structure of the original time series. We demonstrate that this data transformation enables us to apply the fluctuation test and expect reliable results.

Section 2 explains the experimental set-up including the actions to imitate the technical malfunctions and the resulting time series data. In Section 3 we introduce the SCARM and its test for local linearity. Furthermore, we present the new trend-detection procedure and investigate the two methods as to the detection of jumps and (changing) trends by means of simulations and applications to the given time series. In Section 4.1 we introduce the fluctuation test for constant variances. Furthermore, we present the data transformation approach and demonstrate that this transformation makes the test applicable. Section 5 concludes and gives an outlook.

2. Experimental set-up and data

The experiments are conducted using a spray gun of type WokaJet 400[©] from Sulzer Metco with a MultiCoat[©] control module. This module allows a continuous electronic monitoring of several variables. A TWIN 120AH[©] powder feeder provides a permanent powder supply to the hot gas jet by two radial powder injectors. An agglomerated and sintered WC-Co[©] powder with particle sizes between 15 and 45 μm is chosen as feedstock. For all spray plume measurements an AccuraSpray[©] g3 system from Tecnar is employed.

The AccuraSpray[©] g3 provides several different types of data. However, we merely consider the following four variables, since these are known to have great impact on the coating quality [15, 19, 20]:

X^{temp} : the temperature of the spray particles in $^{\circ}\text{C}$,

Table 1. Possible process malfunctions and the actions to imitate them.

Situation	Action to imitate
A: ‘Failure of one powder injector’	Switching off the injector on one side only
B: ‘Pressure drop of the carrier gas’	Lowering the carrier gas pressure by 5%
C: ‘Failure of the air cooling’	Switching off the compressed air supply
D: ‘Worn-out acceleration nozzle’	Replacement of nozzle by a worn-out nozzle ^a

^aSpraying process interrupted to replace the nozzle.

X^{vel} : the particle velocity in m/s,

X^{wid} : the width of the spray jet in mm,

X^{int} : the intensity of the spray jet in %.

The four variables are measured with a frequency of one observation per second over periods ranging from 855 to 904 seconds in four different experiments. The resulting time series are shown in Figures 1 – 4.

The four experiments were run with equal start settings. However, in each experiment the settings are altered after 420 seconds to imitate a certain technical malfunction of the spraying process. Table 1 shows the four considered malfunctions A–D and the actions to imitate them. These malfunctions are likely to occur in practice and can severely affect the spraying process and thus the coating quality.

The effect of the malfunctions is reflected by the time series of the four variables, see Figures 1 – 4. Most of the time series show visible jumps or trends after the malfunction has been imitated, indicating that the process is defective or out of control, respectively.

The situation A: ‘Failure of one powder injector’ is imitated by switching off the injector on one side only. This does not affect the process immediately since the second powder injector is still working. The situation D: ‘Worn-out acceleration nozzle’ is imitated by replacing the well-functioning nozzle by a worn-out nozzle, involving an interruption of the spraying process. Note that a degeneration of the nozzle usually proceeds slowly, yet it is impossible to run the machines until the usual degeneration exceeds a reasonable level. Moreover, the progress of degeneration can usually be described as a steady process that does not show structural changes. Therefore, our statistical analysis of this situation mainly focuses on general differences in the structure of the time series when a well-functioning or a worn-out nozzle is used.

3. The online detection of jumps and (changing) trends

The recently developed *Slope Comparing Adaptive Repeated Median* (SCARM) is a procedure for online filtering (i.e. smoothing) of non-stationary time series [5]. The SCARM fits Repeated Median (RM) regression lines [18] to moving window samples, whose widths are adapted to the current data situation at each time point t . The window width adaption is based on a test for local linearity of the signal, presented in Section 3.1. This test rejects when jumps and trend changes are present and is therefore a promising tool for online break detection. The SCARM test is constructed to detect distinct, sudden changes of the trend, but it cannot detect slight, ongoing trends. Therefore, we develop a new procedure for the online-detection of trends in time series in Section 3.2 which uses the information given by the SCARM. In order to investigate the SCARM and the new trend-detection procedure as to their ability to detect jumps and (changing) trends and as to their

liability to false detections, we determine their *average run lengths* (ARLs) by means of simulations in Section 3.3. Finally, the capabilities of the two procedures are demonstrated by applications to the given time series from thermal spraying processes in Section 3.4.

3.1 The SCARM and its test for local linearity

The SCARM assumes that the observations x_t of the time series (x_t) are drawn from

$$X_t = \mu_t + \varepsilon_t + \eta_t, \quad t \in \mathbb{N}, \quad (1)$$

where μ_t denotes the unknown underlying signal which is smooth but may exhibit sudden jumps and trend changes. Furthermore, ε_t is an error process consisting of independent random variables with zero expectation and time-dependent variance σ_t^2 , and η_t is an outlier process that occasionally generates large absolute values but is zero most of the time. The noise variance σ_t^2 may change over time, but changes of the variance are assumed to occur gradually, so that σ_t can be treated as *locally constant*. That is, even if the fluctuation test from Section 4.1 rejects the hypothesis of constant variance of the *whole* time series, we may apply the SCARM, provided that no sudden variance changes are given. Following the approach of [17], [5] assume that the signal can be approximated well by a line in a short window of size n :

$$\mu_{t-n+i} \approx \mu_t + \beta_t \cdot (i - n), \quad i = 1, \dots, n, \quad (2)$$

where β_t is the slope of the line. Under this assumption of local linearity, the SCARM fits an RM regression line to the window sample $\mathbf{x}_t := (x_{t-n+1}, \dots, x_t)$ by estimating β_t and μ_t :

$$\begin{aligned} \hat{\beta}_t &:= \hat{\beta}(\mathbf{x}_t) = \operatorname{med}_{i \in \{1, \dots, n\}} \left\{ \operatorname{med}_{j \neq i} \left\{ \frac{x_{t-n+i} - x_{t-n+j}}{i - j} \right\} \right\}, \\ \hat{\mu}_t &:= \hat{\mu}(\mathbf{x}_t) = \operatorname{med}_{i \in \{1, \dots, n\}} \left\{ x_{t-n+i} - \hat{\beta}_t \cdot (i - n) \right\}. \end{aligned} \quad (3)$$

The level $\hat{\mu}_t$ is then the estimate of the signal μ_t .

Since the SCARM adapts the size of the window sample \mathbf{x}_t at each time point t , the window width is denoted as n_t in the following. The window width adaption is based on a test for local linearity of the underlying signal $\mu_{t-n_t+1}, \dots, \mu_t$:

$$\begin{aligned} H_0 &: \mu_{t-n_t+i} = \mu_t + \beta_t \cdot (i - n_t), \quad i = 1, \dots, n_t, \\ H_1 &: \mu_{t-n_t+i} = \begin{cases} \mu_t^{\text{old}} + \beta_t^{\text{old}} \cdot (i - n_t), & i = 1, \dots, t_0 \\ \mu_t^{\text{new}} + \beta_t^{\text{new}} \cdot (i - n_t), & i = t_0 + 1, \dots, n_t \end{cases}, \end{aligned}$$

where $t_0 \in \{1, \dots, n_t - 1\}$ and $\mu_t^{\text{old}} \neq \mu_t^{\text{new}}$ and/or $\beta_t^{\text{old}} \neq \beta_t^{\text{new}}$. The alternative H_1 means that a level shift and/or trend change takes place in the time window of size n_t .

In order to perform the SCARM test, the window sample $\mathbf{x}_t \in \mathbb{R}^{n_t}$ is split into two separate parts, the *left-hand sample* $\mathbf{x}_t^{\text{left}} = (x_{t-n_t+1}, \dots, x_{t-r})$ and the *right-hand sample* $\mathbf{x}_t^{\text{right}} = (x_{t-r+1}, \dots, x_t)$, so that $\mathbf{x}_t = (\mathbf{x}_t^{\text{left}}, \mathbf{x}_t^{\text{right}})$. The size r of the right-hand sample is fixed, whereas the size of the left-hand sample is $\ell_t := n_t - r$,

i.e. ℓ_t varies over time. Let \mathbf{X}_t , $\mathbf{X}_t^{\text{left}}$ and $\mathbf{X}_t^{\text{right}}$ denote the referring random vectors, and let $\hat{\beta}_t^{\text{right}} := \hat{\beta}(\mathbf{X}_t^{\text{left}})$ and $\hat{\beta}_t^{\text{left}} := \hat{\beta}(\mathbf{X}_t^{\text{right}})$ denote the *left-hand* and *right-hand RM slopes*, cf. (3). The test statistic of the SCARM is then given by

$$T_t := T(\mathbf{X}_t) = \frac{D_t}{\sqrt{\widehat{\text{Var}}(D_t)}}, \quad D_t := \hat{\beta}_t^{\text{right}} - \hat{\beta}_t^{\text{left}}, \quad (4)$$

where $\widehat{\text{Var}}(D_t)$ is an estimator of the variance of the slope difference D_t from (6), see below. [5] investigate the distribution of the SCARM test statistic T under H_0 and find that it can be approximated well by a t_f -distribution for several error distributions. Hence, [5] reject H_0 if $|T(\mathbf{x}_t)|$ is larger than the $1 - \alpha/2$ -quantile of the t_f -distribution, where the degrees of freedom $f = f(\ell_t, r)$ depend on the sample sizes ℓ_t and r , and α is the level of significance.

Given independent Gaussian errors, the expected number of type I errors, i.e. falsely detected signal changes, in a time series of length N is αN . However, please note that the SCARM test is applied sequentially in moving window samples. In this case, the test should be regarded in an explorative rather than in an inferential sense [21]. Its task is to detect structural breaks in real time to help the engineer or any other process surveillant to decide whether the ongoing process is defective or out of control.

If H_0 is rejected, it is assumed that the underlying signal has changed in the time window. Hence, in this case the window width n_t is set down to a reasonable small value n_{\min} which has to be chosen beforehand. [5] recommend to choose $n_{\min} \approx r/3$ in order to estimate μ_t only on observations that come after t_0 .

If H_0 cannot be rejected, it is justifiable to assume that the signal is (at least approximately) linear in the window of width n_t , so that n_t is not adapted. After the signal has been estimated by fitting the RM line to the window sample of (possibly adapted) width n_t , the new incoming observation x_{t+1} is included into the window sample, so that $n_{t+1} = n_t + 1$. That is, the window width can merely grow gradually, provided that H_0 is not rejected over a period of time. Furthermore, an upper bound n_{\max} for n_t limits the computing time: if $n_{t+1} = n_t + 1 > n_{\max}$, the oldest/leftmost observation of the window sample is excluded, so that $n_{t+1} = n_{\max}$. Afterwards the time index is updated by setting $t \leftarrow t + 1$.

Note that if the window width is set down to a small value n_{\min} at time t^* , at the following time points $t^* + 1, t^* + 2, \dots$ the windows possibly do not contain enough observations for sensible test decisions. Therefore, [5] choose a minimum value ℓ_{\min} for ℓ_t , such that the test is only performed if $n_t \geq \ell_{\min} + r$; [5] recommend to choose $\ell_{\min} = r$. That is, if the test rejects at time point t and $n_{\min} < \ell_{\min} + r$, the test is not performed again until time $t + \ell_{\min} + r - n_{\min}$. For more details about the SCARM-algorithm and the choice of the input arguments $r, \ell_{\min}, n_{\min}, n_{\max}$ and α , see [5].

In order to estimate $\text{Var}(D_t)$, [5] use that

$$\text{Var}(D_t) = \text{Var}(\hat{\beta}_t^{\text{left}}) + \text{Var}(\hat{\beta}_t^{\text{right}}) = \sigma_t^2 \cdot v_\ell + \sigma_t^2 \cdot v_r = \sigma_t^2 \cdot (v_\ell + v_r) \quad (5)$$

under H_0 and given that ε_t is a white noise process. Here v_ℓ and v_r denote respectively the variance of the RM slope for samples of size ℓ and r , where the error follows a specified distribution with variance one. [5] obtain approximations \hat{v}_n by means of simulations using standard normal noise and estimate the error scale σ_t .

Assuming that σ_t is *locally constant*, i.e. constant in the time window of width n_t , [5] estimate σ_t by means of the model-free and robust scale estimator Q^{adj} [12]. The Q^{adj} is applied directly to the data and does not require a preceding regression fit. This leads to a gain in power of the SCARM test since large estimations of $\text{Var}(D_t)$ are prevented [5]. Given a random vector \mathbf{X}_t , the Q^{adj} scale estimator of the noise scale is $\hat{\sigma}_t := Q_\delta^{\text{adj}}(\mathbf{X}_t)$, where

$$Q_\delta^{\text{adj}}(\mathbf{x}_t) = c_n \cdot h_{(t-n+\lfloor \delta(n-2) \rfloor)}.$$

Here $h_{(t-n+\lfloor \delta(n-2) \rfloor)}$ is the δ -quantile of the vertical heights h_{t-n+i} , $i = 2, \dots, n-1$, of the $n-2$ triangles which are built by each triplet of subsequent observations $x_{t-n+i-1}, x_{t-n+i}, x_{t-n+i+1}$:

$$h_{t-n+i} = \left| x_{t-n+i} - \frac{x_{t-n+i-1} + x_{t-n+i+1}}{2} \right|.$$

The factor c_n ensures the unbiasedness of the estimator for a sample of size n with errors coming from a specified distribution. [12] suggest to choose $\delta = 0.5$ to obtain reasonable robustness and efficiency of the Q^{adj} estimator.

[5] obtain approximations \hat{v}_n and constants c_n by means of simulations using standard normal errors. However, if the data are positively (negatively) autocorrelated, these values are too small (too large), so that the proposed estimator

$$\widehat{\text{Var}}(D_t) = c_n \cdot h_{(t-n+\lfloor n/2-1 \rfloor)} \cdot (\hat{v}_l + \hat{v}_r), \quad (6)$$

has a downwards (upwards) bias. We therefore use constants \hat{v}_n^φ and c_n^φ which are obtained by means of simulations on data from an AR(1)-process with parameter $\varphi \in (-1, 1)$ and standard normal error. The constants \hat{v}_n^φ and c_n^φ can then be chosen w.r.t. the parameter φ . Since the thermal spraying time series exhibit autocorrelations at lag one of around 0.6, we use $\varphi = 0.6$ for the application in Section 3.4.

Next, we present a new procedure for the online-detection of trends. This method is based on the fact that at each time point t the SCARM delivers a window width n_t such that the assumption of a linear signal is justifiable.

3.2 A SCARM-based procedure for online trend detection

Our new procedure is based on the same assumptions as the SCARM. We further assume that there is a window width n_t for all t , so that (2) holds exactly:

$$\begin{aligned} \mu_{t-n_t+i} &= \mu_t + \beta_t \cdot (i - n_t) \\ \Leftrightarrow X_{t-n_t+i} &= \mu_t + \beta_t \cdot (i - n_t) + \varepsilon_{t-n_t+i} + \eta_{t-n_t+i}, \end{aligned} \quad (7)$$

with $i = 1, \dots, n_t$. The equivalence is true because of (1), where ε_t denotes the error process with variance σ_t^2 and η_t is the outlier process. If (7) is given, we can interpret β_t as the *current slope* of the signal, and constitute that a trend is given iff $\beta_t \neq 0$. Since the SCARM adapts a window width n_t at each time t , it is justifiable to assume that (7) is true. That is, for all t the SCARM delivers an adequate window width n_t , so that $\hat{\beta}(\mathbf{X}_t)$, the RM slope estimator on $\mathbf{X}_t = (X_{t-n_t+1}, \dots, X_t)$, is

adequate for β_t . We therefore propose the *trend-detection statistic*

$$T_t^* := T^*(\mathbf{X}_t) = \frac{\hat{\beta}(\mathbf{X}_t)}{\sqrt{\widehat{\text{Var}}[\hat{\beta}(\mathbf{X}_t)]}}, \quad (8)$$

where the estimator $\widehat{\text{Var}}[\hat{\beta}(\mathbf{X}_t)]$ is given by

$$\widehat{\text{Var}}[\hat{\beta}(\mathbf{X}_t)] = \hat{\sigma}_t^2 \cdot \hat{v}_{n_t} = c_{n_t} \cdot h_{(t-n_t+\lfloor n_t/2-1 \rfloor)} \cdot \hat{v}_{n_t}$$

in accordance with (5) and (6) and the window width n_t is delivered by the SCARM. Note that the estimator $\widehat{\text{Var}}[\hat{\beta}(\mathbf{X}_t)]$ can be adapted to errors from an AR(1)-process with parameter φ , for instance, by using suitable constants $c_{n_t}^\varphi$ and $\hat{v}_{n_t}^\varphi$, see above.

If a sample \mathbf{x}_t results in a large value of $|T^*(\mathbf{x}_t)|$, we must assume that $\beta_t \neq 0$, meaning that a trend is currently present in the time series (where the sign of $T^*(\mathbf{x}_t)$ indicates the direction of the trend). Similar to the SCARM test one could develop a test procedure based on the trend-detection statistic T_t^* by investigating its distribution under the null hypothesis $\beta_t = 0$. However, if a (test) statistic is computed sequentially in moving window samples of time series observations, it should be regarded as a rather explorative than inferential tool for decision support [21]. Therefore, we refrain from developing a test procedure based on the trend-detection statistic T_t^* from 8. Instead, we suggest to use a decision rule, e.g.

$$R(\mathbf{x}_t) = \begin{cases} 0, & |T^*(\mathbf{x}_t)| \leq c_1 \\ 1, & c_1 < |T^*(\mathbf{x}_t)| \leq c_2, \\ 2, & c_2 < |T^*(\mathbf{x}_t)| \end{cases} \quad (9)$$

where $0 < c_1 < c_2$. Here the situations $R = 0$, $R = 1$ and $R = 2$ could be interpreted respectively as ‘no trend’, ‘warning: slight trend’ and ‘alarm: distinct trend’. Of course also other decision rules could be applied, e.g. using only one threshold $c = 3$, in accordance with the common six-sigma-rule.

The proposed trend-detection procedure offers the same beneficial properties as the SCARM: it is robust against outliers since robust RM regression and robust Q^{adj} scale estimation is used; it only needs negligible small extra computing time since it uses the outputs given by the SCARM; and its algorithm can be implemented easily in an online system so that it is feasible in online practice. We provide an R function of the SCARM-based trend-detection procedure, termed `scarm.detection`, on the website <https://www.statistik.tu-dortmund.de/1543.html>.

3.3 Average run lengths

In the following we investigate the SCARM statistic T_t from Section 3.1 and the trend-detection statistic T_t^* from 3.2 as to their ability to detect structural breaks and their liability to false detections. Results regarding the power of the SCARM test to detect jumps and trend changes can be found in [5]. We determine the *out-of-control* and *in-control average run lengths* (ARLs) of the two procedures. The in-control ARL is the mean time until a break is detected by mistake, and the out-control ARL is the mean time until a given break is detected. The ARLs are determined by simulations using R, version 3.0.1; the simulation programs are available on the website <https://www.statistik.tu-dortmund.de/1543.html>.

Table 2. In-control ARLs of T_t and T_t^* for several types of errors.

Error type	T_t	T_t^*		
		$c = 2$	$c = 3$	$c = 4$
I	1899	311	2017	10771
II	1975	308	1899	10112
III	2920	558	4715	22538
IV	6451	1113	11129	30099
V	5390	742	7830	31728

We apply the SCARM using the R function `scarm.filter` from the R package `robfilter` [9] and choose the input arguments $\alpha = 0.001$, $r = \ell_{\min} = 30$, $n_{\min} = 10$ and $n_{\max} = 200$, in accordance with the suggestions by [5]. The application of the trend detection procedure is carried out using the R function `scarm.detection`, which is provided on the above mentioned website, too.

3.3.1 In-control ARLs

We generate stationary time series $(x_t)_{t \in \mathbb{N}}$ from $X_t = \mu_t + \varepsilon_t$ with $\mu_t = 0$ and independent errors ε_t , considering five types of error distributions:

- Error type I: standard normal errors;
- Error type II: skewed errors from a standardized Weibull distribution with scale and shape parameter two and one;
- Error type III: heavy-tailed errors from a standardized t -distribution with three degrees of freedom;
- Error type IV: errors from a contamination model: $\varepsilon_t \sim 0.9N(0, 1) + 0.1N(10, 1)$;
- Error type V: errors from a contamination model: $\varepsilon_t \sim 0.9N(0, 1) + 0.1N(0, 100)$.

For each error type I–V we generate N time series (x_t) , and for each time series we store the time until $|T_t|$ is larger than the critical value and until $|T_t^*|$ is larger than a certain threshold c . That is, we store the time until a break is detected by mistake. Thus, we can estimate the in-control ARL by the mean of the N respective run lengths, where $N = 1000$ for error type I–III and $N = 500$ for error type IV and V. The results for T_t and for T_t^* with $c = 2, 3, 4$ are shown in Table 2. Apparently, the in-control ARLs of the SCARM and the trend-detection procedure are comparable for the noise types I and II, i.e. for standard normal and skewed Weibull noise. The ARLs for the noise types III–V are larger, i.e. the SCARM rejects less frequently for heavy-tailed or contaminated noise. This is because the Q^{adj} scale estimator from (3.1) has an *explosion breakdown point* of about 1/6 if $\delta = 0.5$, as recommended by [12]. Roughly speaking, this means that the estimator can become arbitrarily large if 1/6 of the observations in a sample are replaced by arbitrarily extreme values. That is, the Q^{adj} estimator is biased upwards due to the extreme observations in the time series with errors of type III–V. Thus, the empirical variances of the statistics T_t and T_t^* are smaller than one, so that their in-control ARLs are longer than the ARLs for standard normal errors.

3.3.2 Out-of-control ARLs

Next we determine the out-of-control ARLs of the trend-detection procedure, i.e. the mean time needed to detect trends with different slopes. We do not present the out-of-control ARLs of the SCARM here as these can be found in [5]. We only remark that, depending on the severity of the break and the chosen input arguments, the out-of-control ARL of the SCARM is roughly about $r/4$ to $3r/4$ time points, where r is the chosen right-hand width.

In order to determine the out-of-control ARL of the trend-detection procedure,

Table 3. Out-of-control ARLs of T_t^* for trends with slope b .

b	$c = 2$	$c = 3$	$c = 4$	b	$c = 2$	$c = 3$	$c = 4$
0.01	57.6	87.1	111.0	0.1	18.7	26.2	33.2
0.02	40.9	58.9	73.2	0.2	12.3	16.9	20.2
0.03	33.8	48.6	60.4	0.3	10.0	12.7	14.9
0.04	29.8	43.1	53.7	0.4	8.6	10.7	12.3
0.05	26.7	38.6	48.6	0.5	7.9	9.5	10.8
0.06	24.2	35.3	45.1	0.6	7.6	8.8	9.8
0.07	22.6	32.4	41.7	0.7	7.3	8.4	9.2
0.08	21.1	30.5	38.1	0.8	7.1	8.2	8.8
0.09	19.7	28.2	35.7	0.9	7.0	8.1	8.6
0.10	18.7	26.2	33.2	1.0	6.9	7.9	8.5

we generate time series (x_t) from $X_t = \mu_t + \varepsilon_t$, where $\varepsilon_t \sim N(0, 1)$ and

$$\mu_t = \begin{cases} 0, & t = -n, -n + 1, \dots, 0 \\ b \cdot t, & t = 1, 2, \dots \end{cases}.$$

That is, for the first n observations the time series is stationary, and then at time $t = 1$ a trend of slope b starts. Here n is the width the SCARM uses to estimate the slope and level at time $t = 0$. The width n is chosen with equal probability from $\{10, 11, \dots, 200\}$ in order to imitate the situation in practice, as the size of the window sample to compute T_t^* is chosen automatically by the SCARM. We generate 1000 time series for $b \in \{0.01, 0.02, \dots, 0.1, 0.2, \dots, 1\}$ and store the time until $|T_t^*| > c$, considering the thresholds $c = 2, 3, 4$. Hence, we obtain 1000 detection times for each slope b and each threshold c , so that the out-of-control ARLs can be estimated by the mean of the 1000 respective detection times. Table 3 presents the results. As was to be expected, the out-of-control ARLs decrease with increasing b and decreasing c . That is, distinct trends are detected earlier than slight trends, and a small threshold c induces a short out-of-control ARL – but at the cost of a short in-control ARL, see Table 2. Anyway, the obtained in-control and out-of-control ARLs demonstrate the capabilities of the SCARM and the new trend detection procedure, as they offer long in-control ARLs and short out-of-control ARLs.

3.4 Application of the SCARM test and the trend-detection procedure

Next we apply the SCARM and the trend-detection procedure to the four time series (x_t^{temp}) , (x_t^{vel}) , (x_t^{wid}) and (x_t^{int}) for each of the four situations A–D listed in Table 1 in order to investigate their performances as to the online-detection of the existent structural breaks. The SCARM is applied using R, version 3.0.1, and the R function `scarm.filter` from the package `robfilter` [9]. The application of the trend detection procedure is carried out using the R function `scarm.detection`, which can be downloaded on the website <http://www.statistik.tu-dortmund.de/1543.html>. Both R functions are applied offline here, yet an online application would deliver the same results.

[5] recommend to choose a small significance level α for the SCARM test, as one expects one type I error every $1/\alpha$ time points under H_0 . Since [5] find that the SCARM test yields good power also for small levels of significance, we use $\alpha = 0.001$. Furthermore, we use the input arguments $\ell_{\min} = r = 40$, $n_{\min} = \lfloor r/3 \rfloor = 13$ and $n_{\max} = 200$, which is in accordance with the recommendations by [5]. The trend-detection procedure is applied using the decision rule (9) with $c_1 = 2$ and $c_2 = 4$.

Since the data are rounded to one decimal place, ties are likely to occur in the

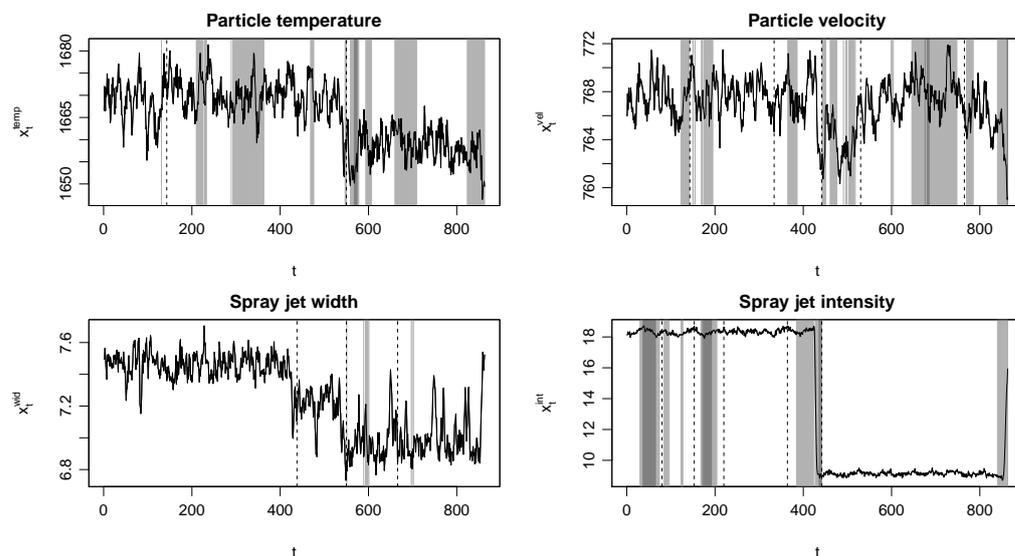


Figure 1. Time series (x_t^{temp}) , (x_t^{vel}) , (x_t^{wid}) and (x_t^{int}) for situation A: ‘Failure of one powder injector’; signal changes detected by the SCARM test are marked by vertical lines.

window samples. Ties can cause that the Q^{adj} estimator becomes zero, so that the R functions give infinite values of the statistics T_t and T_t^* . Therefore, we ‘wobble’ the data [8] by adding white noise from a normal distribution with zero mean and variance ς^2 . In each situation A–D and for each of the four time series, we choose ς equal to half of the empirical standard deviation of the first 400 observations of the transformed time series (\tilde{x}_t) from Section 4.1. Due to the wobbling there are no more ties in the data, yet signal changes are not covered by noise since the wobbling scale is small enough.

The Figures 1 – 4 display the time series (x_t^{temp}) , (x_t^{vel}) , (x_t^{wid}) , (x_t^{int}) for each of the four situations A–D. The time points of jumps of trend changes detected by the SCARM test are marked by black vertical dashed lines. The time points when the trend-detection procedure decides respectively for $R = 1$: ‘warning: slight trend’ and $R = 2$: ‘alarm: distinct trend’ are marked by vertical lines colored in light-grey and dark-grey.

Due to the failure of one powder injector (Figure 1) at time $t = 420$, jumps occur respectively around $t = 420$ in the time series (x_t^{vel}) , (x_t^{wid}) and (x_t^{int}) and around $t = 550$ in the time series (x_t^{wid}) and (x_t^{temp}) . Obviously, this malfunction has a delayed effect on the temperature of the spraying process and an immediate effect on the remaining variables. The SCARM test detects all the provoked changes immediately. It also detects some further signal changes, where most of these decisions are comprehensible but some of them must be regarded as type I errors, i.e. false detections. Using the trend-detection statistic T_t^* we detect slight trends in all four time series. However, most of these ‘slight-trend-periods’ are rather short, indicating that these are false detections in the sense of type I errors.

The time series for the situations B: ‘Pressure drop of the carrier gas’ (Figure 2) and C: ‘Failure of the air cooling’ (Figure 3) show some similarities. In both cases B and C, the series (x_t^{vel}) and (x_t^{int}) do not exhibit jumps or apparent trend changes when the malfunctions are induced. The SCARM test detects some slight changes at other time points, but these detections can be regarded as irrelevant warnings in the sense of type I errors. Since in both cases B and C the time series (x_t^{vel}) and (x_t^{int}) show ongoing negative trends, the trend-detection statistics T_t^* correctly indicate longer time periods of slight or distinct trends. This is also the case for the time series (x_t^{temp}) in situation B. Furthermore, it seems that the manipulations B

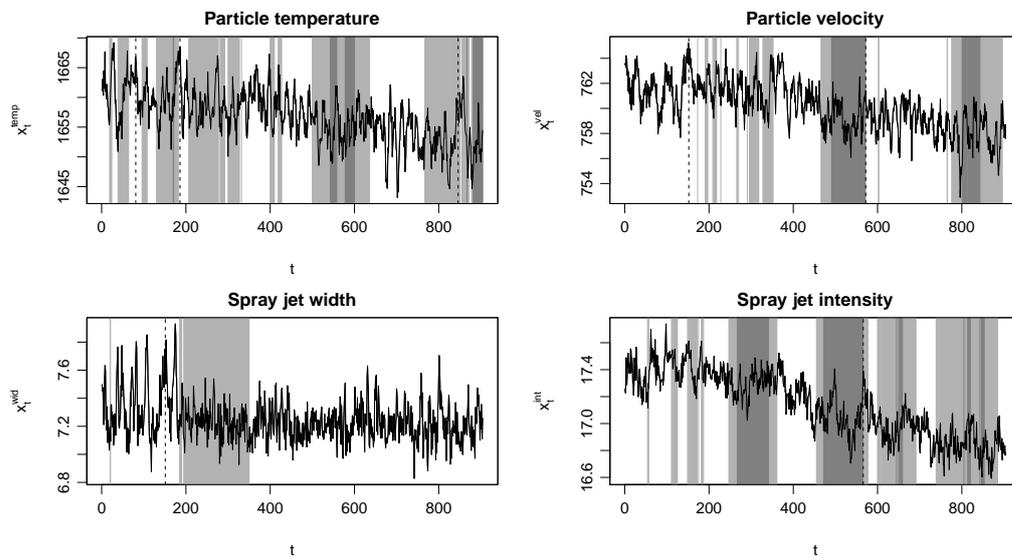


Figure 2. Time series (x_t^{temp}) , (x_t^{vel}) , (x_t^{wid}) and (x_t^{int}) for situation B: ‘Pressure drop of the carrier gas’; signal changes detected by the SCARM test are marked by vertical lines.

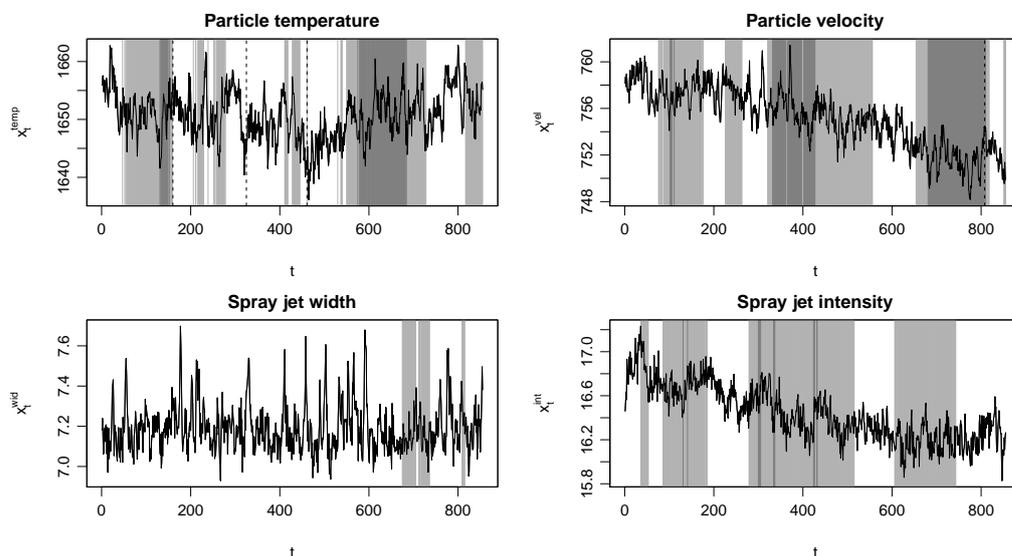


Figure 3. Time series (x_t^{temp}) , (x_t^{vel}) , (x_t^{wid}) and (x_t^{int}) for situation C: ‘Failure of the air cooling’; signal changes detected by the SCARM test are marked by vertical lines.

and C do not affect the spray jet width X^{wid} . The SCARM detects only one signal change in (x_t^{wid}) for situation B, and the trend-detection statistics T_t^* display short periods of slight trends in both situations B and C. However, these detections are rather false decisions in the sense of type I errors.

In situation C, the particle temperature time series is quite unstable, showing jumps and trends. The SCARM detects three jumps, including the jump induced by the provoked malfunction, and there are two periods when the trend-detection procedure gives alarms due to distinct trends.

In situation D (Figure 4), the time series (x_t^{temp}) , (x_t^{vel}) and (x_t^{int}) exhibit slight positive trends and a distinct jump caused by the provoked malfunction. The trends are indicated by the trend-detection procedure, and the jumps are detected immediately by the SCARM. The time series of the spray jet width (x_t^{wid}) differs remarkably from the other three series. It shows two distinct jumps that are detected

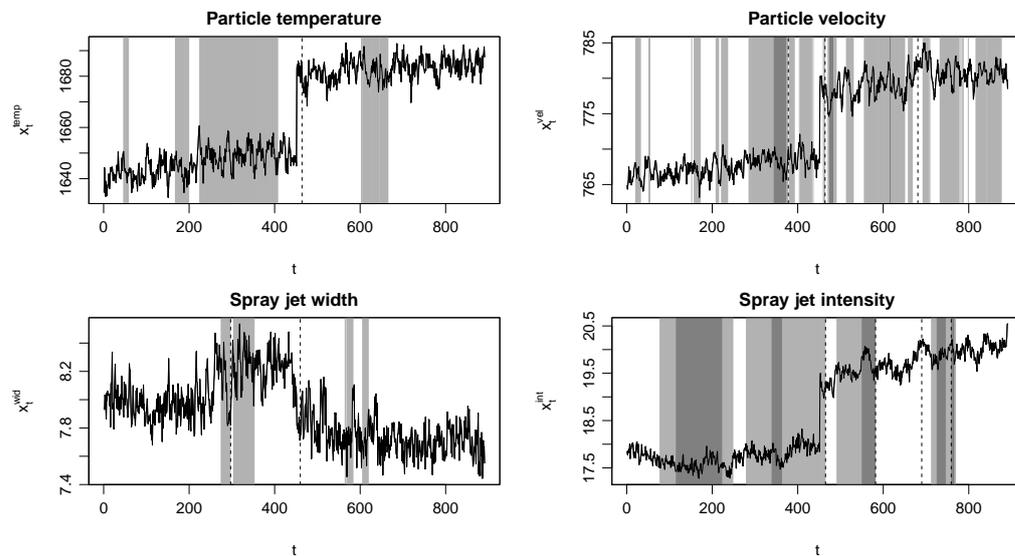


Figure 4. Time series (x_t^{temp}) , (x_t^{vel}) , (x_t^{wid}) and (x_t^{int}) for situation D: ‘Worn-out acceleration nozzle’; signal changes detected by the SCARM test are marked by vertical lines.

by the SCARM. The trend-detection procedure indicates slight trends, yet these decisions can be regarded as irrelevant warnings, also because the warning periods are rather short.

Finally, we point out that the SCARM detects all structural breaks that are caused by all deliberately induced malfunctions. Yet it also detects more than the provoked structural breaks. However, false or irrelevant detections are unavoidable, especially if tests are applied sequentially in moving window samples. Altogether the SCARM made about 20 type I errors. Given a total of 14052 time series observations the type I error rate is $20/14052 \approx 0.0014$. This complies with the chosen level of significance $\alpha = 0.001$.

4. A fluctuation test for constant variances

The recently developed fluctuation test by [22] offers the opportunity to detect changes in the variance of time series. However, the fluctuation test requires weak stationarity of the series. If this assumption is not fulfilled due to jumps and trends (as is the case in the thermal spraying application due to the conducted manipulations), the test tends to reject the null hypothesis, even if a constant variance is given. Therefore, we transfer the original non-stationary time series into time series which can be assumed to be mean-stationary and which reproduce the variabilities of the original time series. Using this transformation we are able to apply the fluctuation test and can expect reliable results.

In Section 4.1 we present the fluctuation test and its properties. In Section 4.2 we demonstrate how jumps affect the outcome of the fluctuation test and present the data transformation. The fluctuation test is applied to the transformed time series of the particle properties in Section 4.3.

4.1 The fluctuation test and its properties

Given a sequence of random variables $(X_t, t \in \mathbb{N})$, which are assumed to have finite absolute $(4 + \delta)$ th moments, $\delta \in \mathbb{R}$, the test problem of the fluctuation test for

constant variances is

$H_0 : \text{Var}(X_1) = \dots = \text{Var}(X_T)$ vs. $H_1 : \exists t \in \{1, \dots, T-1\} : \text{Var}(X_t) \neq \text{Var}(X_{t+1})$.

The corresponding test statistic is

$$Q_T(X) = \max_{1 \leq j \leq T} \left| \hat{D} \frac{j}{\sqrt{T}} ([\text{Var}X]_j - [\text{Var}X]_T) \right|, \quad (10)$$

where

$$[\text{Var}X]_l = \frac{1}{l} \sum_{t=1}^l X_t^2 - \left(\frac{1}{l} \sum_{t=1}^l X_t \right)^2 =: \overline{X_l^2} - (\overline{X_l})^2$$

is the empirical variance calculated from the first l observations. Furthermore, we have

$$\hat{D} = \left((1, -2\overline{X_T}) \hat{D}_1 (1, -2\overline{X_T})' \right)^{-1/2}$$

with

$$\hat{D}_1 = \frac{1}{T} \sum_{t=1}^T \hat{U}_t \hat{U}_t' + 2 \sum_{j=1}^T k \left(\frac{j}{\sqrt{T}} \right) \frac{1}{T} \sum_{t=1}^{T-j} \hat{U}_t \hat{U}_{t+j}'$$

and

$$\hat{U}_t = \begin{pmatrix} X_t^2 - \overline{X_T^2} \\ X_t - \overline{X_T} \end{pmatrix}, \quad k(x) = \begin{cases} 1 - |x|, & |x| \leq 1 \\ 0, & \text{else} \end{cases}.$$

The test rejects the null hypothesis if the empirical variances fluctuate too much over time. In order to derive a limiting null distribution the following assumptions have to be stated, see [22]:

- (A1) The sequence $(X_t, t \in \mathbb{N})$ is weak-sense stationary.
- (A2) For

$$U_t = \begin{pmatrix} X_t^2 - \mathbb{E}(X_1^2) \\ X_t - \mathbb{E}(X_1) \end{pmatrix}$$

and $S_j = \sum_{t=1}^j U_t$, we have

$$\lim_{T \rightarrow \infty} \mathbb{E} \left(\frac{1}{T} S_T S_T' \right) =: D_1 \text{ is finite and positive definite.}$$

- (A3) The r -th absolute value of the components of U_t are uniformly bounded for some $r > 2$.

- (A4) The sequence $(X_t, t \in \mathbb{N})$ is L_2 near-epoch dependent with size $-r-1/r-2$, with r from (A3), and constants (c_t) on a sequence $(V_t), t \in \mathbb{N}$, which is α -mixing of size $\phi^* := -r/r-2$, such that

$$c_t \leq 2 \left(\mathbb{E}|X_t^2 - \mathbb{E}(X_1^2)|^2 + \mathbb{E}|X_t - \mathbb{E}(X_1)|^2 \right)^{\frac{1}{2}}.$$

Table 4. Empirical type I error.

τ	$\hat{\alpha}_\tau$	$\hat{\alpha}_\tau$ with filtering		
		$n = 11$	$n = 31$	$n = 51$
0.5	0.18	0.029	0.029	0.037
2	1	0.032	0.030	0.027
5	1	0.019	0.007	0.001

The limiting null distribution of the test statistic Q_T can now be stated in the following theorem, see [22].

THEOREM 4.1 *Under H_0 and given (A1) to (A4) we have*

$$Q_T(X) \rightarrow \sup_{z \in [0,1]} |B(z)|,$$

where $B(z)$ is a one dimensional Brownian bridge.

Theorem 4.1 allows to determine quantiles of the null distribution in order to apply the test. The quantiles for the null distribution are 1.224 for $\alpha = 0.1$, 1.358 for $\alpha = 0.05$ and 1.628 for $\alpha = 0.01$.

[22] study the asymptotic local power of the test which is always larger than or equal to α under certain conditions. Furthermore, they investigate the power for different sample sizes and different variances in the first and second half of the time series by means of Monte Carlo studies. The empirical power reaches values of at least 0.886 already for a sample size of 800. It is basically observed that the power increases with the sample size.

The fluctuation test can be used to assess the outcome of the thermal spraying process by testing the observed time series of the particle properties for constant variance. If the test rejects, the engineer should check the spraying result. However, we cannot expect the fluctuation test to deliver reliable results for the given thermal spraying time series since these exhibit jumps and therefore do not fulfill the assumption of weak-sense stationarity (A1), see Figures 1 – 4. In the following we demonstrate how jumps affect the fluctuation test and present a data transformation approach that makes the test applicable.

4.2 The fluctuation test for non-stationary time series

In order to demonstrate that jumps affect the fluctuation test, we conduct a small simulation study using R 3.0.1. The R programs are available on the website <https://www.statistik.tu-dortmund.de/1543.html>. We generate 1000 time series of 1000 standard normal distributed values x_1, \dots, x_{1000} and add $\tau \in \{0.5, 2, 5\}$ to x_{501}, \dots, x_{1000} , so that a jump is present at time point $t = 501$. For all $\tau = 0.5, 2, 5$, we apply the fluctuation test with level of significance $\alpha = 0.05$ to the 1000 different series, obtaining 1000 test decisions for each τ . The empirical type I errors $\hat{\alpha}_\tau$ are then the numbers of (false) rejections divided by 1000. These are presented in Table 4, second column. The rate of empirical type I errors clearly exceeds the chosen level of significance of 0.05 with $\hat{\alpha}_\tau = 0.18$ for the small jump of height $\tau = 0.5$ and $\hat{\alpha}_\tau = 1$ for the larger jumps of height $\tau = 2$ and $\tau = 5$.

Obviously, the fluctuation test for constant variances is not reliable when jumps and trends are present in the time series. However, if the ‘signal-plus-noise-assumption’ (1) was true and the underlying signal μ_t was known for all t , we could subtract μ_t and obtain a mean-stationary time series (with zero mean) that would offer the same (possibly changing) variability as the original time series, cf. Appendix A. However, although the presence of an underlying signal is a com-

mon and justifiable assumption in many applications, the signal itself is generally unknown, i.e. μ_t must be estimated for all t .

The signal μ_t could be estimated by the SCARM from Section 3.1. However, the SCARM estimate $\hat{\mu}_t$ is the level of the RM regression line at the rightmost position of the moving time window, because this point equates to the current time point in an online application. Although this approach results in a ‘full-online’ signal estimation, the course of the signal is traced with a certain time delay. That is, the SCARM estimates $\hat{\mu}_t$ differ considerably from the true μ_t after jumps and trend changes [5]. Hence, the SCARM is a rather improper method for our purpose. However, since we want to apply the fluctuation test offline, we actually do not need a ‘full-online’ signal estimation. Instead, we use a retrospective signal estimation approach and fit RM regression lines to a moving window of odd width $n = 2w + 1$ [7, 11]. The level of the regression line at the central window position $w + 1$ is then the signal estimate at the referring time point t . We explain this offline signal estimation in detail in Appendix A.

The positive effect of the data transformation is demonstrated in Table 4. Here the third column contains the empirical type I errors of the fluctuation test applied to the time series transformed by RM signal estimation with $n = 11, 31, 51$. The empirical type I errors are lower than the significance level $\alpha = 0.05$ for each window width n , i.e. the test keeps the chosen level of significance if the time series are transformed to mean-stationarity beforehand.

4.3 Application of the fluctuation test

Although the proposed data transformation helps to keep the level of significance, we have to bear in mind that the chosen width n of the moving window can have large impact on the signal estimation and thus on the resulting transformed time series. That is, the results of the fluctuation test may depend on the chosen window width n . Therefore, we apply the fluctuation test to the RM-transformed time series $(\tilde{x}_t^{\text{temp}})$, $(\tilde{x}_t^{\text{vel}})$, $(\tilde{x}_t^{\text{wid}})$ and $(\tilde{x}_t^{\text{int}})$ in each situation A–D using several different window widths n for the RM-transformation. The applications are carried using R, version 3.0.1; the R program is available on the website <https://www.statistik.tu-dortmund.de/1543.html>. Figure 5 displays the results of the fluctuation tests in situations A–D for $n \in \{11, 21, \dots, 201\}$. The solid horizontal line marks the 0.95-quantile of the null distribution of the fluctuation test. Figure 5 shows that in most cases the null hypothesis cannot be rejected at the 0.05-level, meaning that we cannot detect a change in the variance of the time series. However, the test rejects the null hypothesis for $(\tilde{x}_t^{\text{wid}})$ in the situations A and B (except for $n = 11, 21$ in situation B). One might therefore suppose that a failure of one powder injector (situation A) or a pressure drop of the carrier gas (situation B) involve a change of the variance of the spray jet width. However, the time series $(\tilde{x}_t^{\text{wid}})$ for the situation B (Figure 2) do not indicate that the variance change is caused by the manipulation. A change is detected rather because of the large fluctuations at the beginning of the time series.

Furthermore, Figure 5 indicates that the test results are independent of the chosen window width n : The fluctuation test rejects the null hypothesis of a constant variance at the 0.05-level either for all or for no values of n . The only exception is the width of the spray jet in situation B. Here the test does not reject for $n = 11, 21$ but for all other values of n . This is because the signal estimates of the RM-filter resemble the original data if n is small. Hence, the transformed time series do not reproduce the large fluctuations at the beginning of the original time series. Due to this finding, we recommend not to choose a too small window width n .

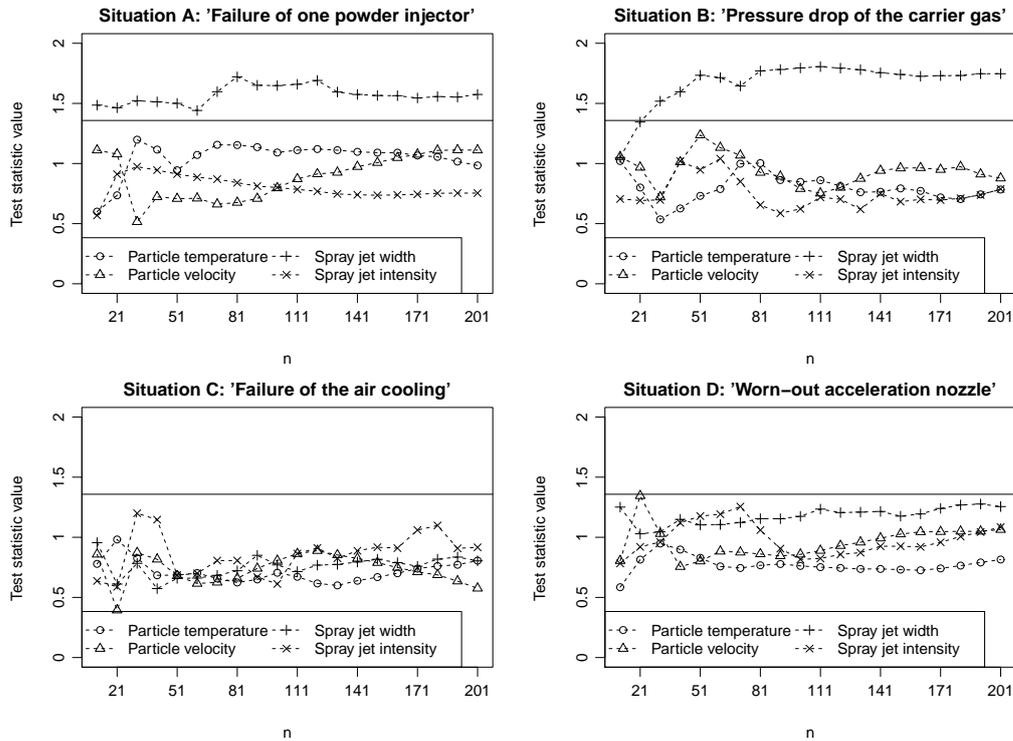


Figure 5. Results of the fluctuation tests applied to the RM-transformed time series $(\hat{x}_t^{\text{temp}})$, (\hat{x}_t^{vel}) , (\hat{x}_t^{wid}) and (\hat{x}_t^{int}) using $n \in \{11, 21, \dots, 201\}$ for the situations A–D; the solid horizontal line marks the 0.95-quantile of the null distribution.

5. Conclusion and outlook

We investigate and develop methods to find structural changes on- and offline in time series of thermal spraying processes. Since technical malfunctions were deliberately induced during the processes, we know that the time series exhibit structural breaks and also when these breaks occur. We consider three methods:

First, the SCARM test by [5] for the online detection of jumps and trend changes; second, a newly developed SCARM-based procedure for the online detection of trends in time series; third, a fluctuation test by [22] for the offline detection of changes in the variance. The new procedure for the online-detection of trends in time series uses the output information given by the SCARM in order to estimate the slope of the current trend. A simple decision rule is used to decide at each time point t whether there is a (slight/distinct) trend or not.

We determine the in-control and out-of-control average run lengths (ARLs) of the SCARM and the trend-detection procedure by means of simulations. The ARLs indicate the capabilities of the two methods as they offer short out-of-control and long in-control ARLs in all considered situations. The applications of the SCARM and the trend-detection procedure to the given time series from thermal spraying confirm these findings.

The fluctuation test for constant variance assumes the weak stationarity of the time series, which is in fact not fulfilled for the given time series due to the structural breaks. We demonstrate that the empirical rates of type I errors of the fluctuation test clearly exceed the level of significance if jumps are present. Therefore, we suggest data transformation based on signal estimation by robust regression in a moving time window of width n . The transformed time series can be regarded as mean-stationary and reproduce the possibly changing variability of the original

data. We demonstrate that the test keeps the level of significance if it is applied to the transformed data so that we can expect reliable results. Furthermore, we find that the influence of the window width n on the test results is negligible provided that n is not unreasonable small.

The combination of the SCARM and the trend-detection procedure can be a useful tool for the online-surveillance of thermal spraying processes, but also for monitoring time series from any other kind of production process. When a warning or an alarm is given, the process surveillant can check and react if necessary. Hence, production failures could be avoided. Furthermore, the fluctuation test can be applied for a final quality control of the production results after the process is finished. If the test rejects the null hypothesis of a constant variance, the product requires a closer inspection.

The thermal spraying processes have been monitored by measuring four variables: the temperature and velocity of the spray particles and the width and intensity of the spray jet. Since there are apparent dependencies between the four time series, a multivariate (online or offline) analysis would be promising. A multivariate version of the SCARM already exists [4], and the development of a multivariate extension of the fluctuation test by [22] is an interesting task for further research. We intend an analysis of the given time series with these and other multivariate methods (see [1], for instance) for future research, including a comparison with the results from the univariate analysis conducted here.

Acknowledgements

The financial support of the Deutsche Forschungsgemeinschaft (SFB 823, projects A1, B1 and C1) is gratefully acknowledged.

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Appendix A. Signal estimation by robust Repeated Median regression

The *signal estimation* or *filtering* is based on the assumption that the data x_t come from an unknown signal μ_t , which is disturbed by an error process ε_t :

$$X_t = \mu_t + \varepsilon_t, \quad t \in \mathbb{N}.$$

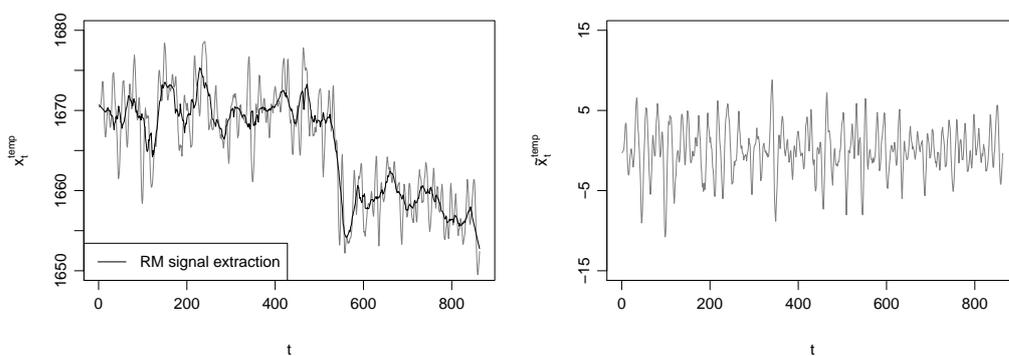


Figure A1. Left plot: original time series (x_t^{temp}) for situation A: ‘Failure of one powder injector’ (grey) and RM signal estimation (black). Right plot: resulting RM-transformed time series $\tilde{x}_t^{\text{temp}}$.

It is assumed that the signal is ‘smooth’ but might also show sudden jumps or trend changes. The noise process has zero mean and time-dependent variance σ_t^2 . The idea is to estimate the signal and to subtract the signal estimate $\hat{\mu}_t$ from the original data:

$$\tilde{x}_t = x_t - \hat{\mu}_t.$$

Let \tilde{X}_t denote the random variable corresponding to \tilde{x}_t . Given that $\hat{\mu}_t = \mu_t$ for all $t \in \mathbb{N}$, it is

$$E(\tilde{X}_t) = 0 \quad \text{and} \quad \text{Var}(\tilde{X}_t) = \text{Var}(X_t) = \sigma_t^2, \quad (\text{A1})$$

for all $t \in \mathbb{N}$, i.e. the time series (\tilde{x}_t) is mean-stationary with zero mean and has the same (possibly changing) variability as the original time series (x_t). Hence, provided that the signal estimation $\hat{\mu}_t$ is adequate, it is justifiable to assume that (A1) holds.

[7, 11] estimate the signal μ_t by fitting regression lines to moving window samples ($x_{t-w}, \dots, x_t, \dots, x_{t+w}$) of width $n = 2w + 1$:

$$\hat{\mu}_{t+i} = \hat{\mu}_t + \hat{\beta}_t \cdot i, \quad i = -w, \dots, w,$$

where $\hat{\beta}_t$ is the slope of the regression line and $\hat{\mu}_t$, the level at the central window position t , is the estimate of the signal μ_t . We follow the suggestions of [7, 11] and use robust Repeated Median (RM) regression [18] to obtain the signal estimation series ($\hat{\mu}_t$) and thus the transformed time series (\tilde{x}_t). This is done by means of the R-function `rm.filter` from the package `robfilter`, version 4.0, [9]. Figure A1 presents an exemplary application of the RM filter to the time series (x_t^{temp}) for the situation A: ‘Failure of one powder injector’. The left plot shows the original time series (grey) and the RM signal estimation (black). The right plot shows the resulting RM-transformed series ($\tilde{x}_t^{\text{temp}}$) using $n = 31$. Obviously, the variability of the original time series is reproduced by the RM-transformed time series, yet the RM-transformed time series can be assumed to be mean-stationary in contrast to the original series. Therefore, we can expect reliable results applying the fluctuation test to the RM-transformed time series (\tilde{x}_t) — in contrast to applying the test to the original non-stationary time series (x_t).