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Selection of Signal Processing Techniques for Extracting Quantitative Indicators of Paste Quality from Extrusion Pressure Data

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Signal processing techniques have been developed for extracting quantitative indicators of the performance of extruders processing soft-solid pastes from the data recorded by pressure transducers located near the extrusion die. Such techniques have been applied previously to isothermal ram and screw devices using retrospective methods. This article reports on the scope for application of retrospective algorithms, ideally suited to ram extrusion, to continuous systems. Novel Bayesian methods for the detection of outliers were found to be unsuitable for real-time analysis, prompting the development of a gradient-based algorithm. A number of fractal analysis techniques for quantifying the paste homogeneity were assessed and proved to be less robust than indicators based on coefficient of variance. Periodic variations related to acute, circumferential fracture were readily identified by a Bayesian model-based approach. Application to practical systems is illustrated by tests on several different paste materials following theoretical investigations on numerically generated data.

Keywords Control; Extrusion; Fracture; Homogeneity; Paste; Signal processing

Introduction

The manufacture of shaped semisolid products via paste extrusion is becoming an increasingly important technology in industry. The main industrial modes of forming are by ram extrusion, where the material is presented to the die by a moving piston, and auger extrusion, where the material is fed by rotating screws. Pastes are soft-solid materials, and simple examples consist of highly filled suspension of particulate solids (with a typical size range between 1 and 100 μm) and a liquid binder phase (Benbow and Bridgwater, 1993), such that the material can be molded readily, but still be stiff enough that it retains its shape in the absence of applied forces.

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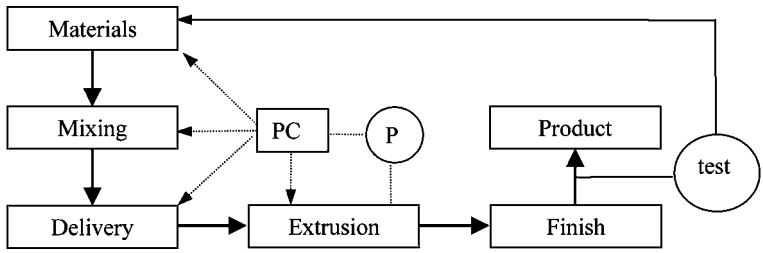


Figure 1. Advantages of a pressure signal processing approach (dashed line) over conventional test-based control (solid line).

Pastes often feature solids volume fractions in excess of 60% (Blackburn, 1995), so that interparticle contacts dominate the rheology of these materials at low strain rates and give rise to yield stress behavior. They can exhibit viscoplastic, elastic, and thixotropic behavior, depending on the nature of the liquid phase, interparticle packing, and time scale of deformation. Paste extrusion behavior is intimately linked to microstructure as this both dictates the occurrence of processes such as liquid phase redistribution (Rough et al., 2000) and particle de-agglomeration (Reed, 1993), and determines the performance and quality of the extrudate product.

Microstructural variation and defects in the paste matrix, such as agglomerates, can have adverse effects on the quality of the extrudate without noticeably changing the thermo-mechanical performance of the process. The most common types of extrusion defects are internal cracks and surface fracture, which have an adverse effect on the strength of the final product (Domanti et al., 2002). Manufacturing units often employ statistical process control (SPC) for process assurance, but these methods are not usually aimed at identifying fine-scale or short-term disturbances related to variations in extrudate quality. Quality monitoring frequently relies on time-consuming batch testing at the end of the process, as shown schematically in Figure 1, resulting in long and information-poor feedback loops. It is therefore desirable to determine whether such features can be detected by other means, preferably on-line, in order to allow corrective actions to be implemented.

Amarasinghe and Wilson (1998) studied the fluctuations in pressure measurements obtained from transducers located at or near the die during isothermal ram extrusion of pastes through simple geometry dies and used a range of signal processing techniques to extract useful information related to defect phenomena in the paste. Their work indicated that the use of appropriate signal processing techniques can yield indicators of defect factors in real-time, leading to significantly shorter feedback loops, containing more specific information about the material being processed. They later (Amarasinghe and Wilson, 1999) reported three groups of methods for analyzing pressure transducer data, relating particular trends to different defect behaviors in the paste, thereby laying the basis for monitoring, and ultimately controlling, paste processing. Their methods were:

(i) Outlier analysis, detecting the presence of air pockets and agglomerates in the paste.
(ii) Standard error and fractal analysis, indicating the overall homogeneity of the paste.
(iii) Spectral analysis, identifying and measuring periodic forces related to surface fracture.

Russell et al. (2003) subsequently reported the development of more robust signal processing techniques, which were applied to the ram extrusion of a range of different paste materials. Extension of these techniques to continuous operations (e.g., auger extruders) was demonstrated successfully by Russell et al. (2004), albeit again on a retrospective basis, where data were collected over a period and analyzed off-line.

On-line implementation of this methodology requires identification of fast retrospective methods or the development of continuously updating algorithms that could be applied on a real-time basis without intensive computational need. This article presents an evaluation of a range of routines, with particular focus on continuous applications; comparison with previously reported methods is included to compare their effectiveness and demands on computation. Particular attention is given to fractal techniques, which have been shown to be useful for other particulate systems characterized by random contacts (Kwon et al., 1994).

This work considers near-isothermal extrusion through simple, concentric dies where disturbances chiefly arise from the material being processed; it is recognized that multi-holed dies and intricately shaped systems will generate more complex data patterns owing to flow variations driven by variability in material consistency. In a similar vein, temperature effects are acknowledged to be important, particularly where the components exhibit phase changes over the operating conditions where temperature can be monitored directly, this information could be combined with the pressure data methodology described here to assess operation. Process conditions such as ram or screw speed, which affect the rate of extrusion, do not have a direct effect on quality, as long as the sampling time scales are correctly selected and transducer response times are not infringed upon. Ram and screw speed can, however, exert indirect effects in systems where viscous dissipation or shear dependent ordering induces material transformation. An example is the cold extrusion of chocolate, where shear work induces localized melting of fat (Mulji et al., 2003; Russell et al., 2005) components.

Several different pastes have been used as the basis for this study, partly to ensure that any quality monitoring methods are not peculiar to a single material and also to illustrate the effect that different microstructures and rheologies have on signals gathered. This is a major theme of the work in terms of homogeneity and will be covered later.

Experimental Data

The signal processing results presented here were obtained from analysis of experimental data sets generated by tests on ram extrusion and twin-screw extrusion devices. A full description of experimental protocols, paste materials, and data logging specifications can be found in previous articles (Russell et al., 2003, 2004), as can a rheological characterization of the pastes by the Benbow-Bridgwater method (1993). Three different pastes were processed to establish applicability of the signal processing techniques to a range of paste systems: a model α-alumina ceramic paste, termed Mix 25; a clay-based detergent paste provided by Procter & Gamble Technical Centre, Newcastle-upon-Tyne, UK; and a cohesive potato starch dough provided by United Biscuits, High Wycombe, UK. Details of the paste formulations are given by Russell et al. (2003). All three pastes exhibited strongly viscoplastic rheologies and wall slip.

The ram extrusion system featured a 25 mm diameter vertical cylindrical barrel with concentric circular dies of various diameters and length located at its base. The system was positioned on a computer-controlled strain frame, with the crosshead driving the ram at a set velocity. The premixed paste was packed into the barrel, consolidated to expel air, and then extruded. Solid-state pressure transducers (Kulite, Basingstoke, UK) were positioned in the die.

Screw extrusion experiments were performed on a Haake Rheomex PTW25p unit (Karlsruhe, Germany) with barrel dimensions 16 mm diameter × 390 mm length, fitted with both conveying and kneading sections. Powder components were fed from a vibrating hopper and the liquid phase (in this case, water) injected at separate ports. A pressure transducer was located at the end of the barrel, just before the die entrance. In addition to these pressure measurements, the torque applied to the screws and temperature at various points along the barrel could be recorded at 1 Hz.

Data were collected at sampling speeds of typically 100 Hz to avoid mains aliasing in both ram and screw extrusion. Both ram and screw extrusion modes yielded contained systematic process or instrument components in the pressure signal that needed to be removed in order to study the true process-related fluctuations. The pressure transducer noise was a significant presence in both cases, particularly at high frequencies; in retrospective studies this was removed using a standard discrete wavelet transform (Russell et al., 2003). Additionally, the screw elements in the continuous system presented significant sinusoidal components, which were filtered out in the frequency domain using conventional Fourier methods on a retrospective basis (Russell et al., 2004).

The results from the signal processing were compared to physical attributes of the extrudates, including water content, density, appearance, and mechanical strength, the latter being obtained from a three-point bending test on the dried extrudate prior to any finishing process. Details of these tests are given by Russell et al. (2004).

Outlier Analysis

Pits in the pressure signal represent one type of outlier encountered in extrusion data, and these correspond to the bursting of pockets of entrapped air. Amarasinghe and Wilson (1998) ram-extruded a ceramic paste into a sound-insulated box containing a microphone so that pressure and sound signals could be recorded simultaneously. Sound events corresponding to bursting of air pockets (peaks in the microphone signal) were coincident with the pits in the pressure signal, therefore confirming the above hypothesis. The other type of outlier is a spike, a localized increase in pressure, indicative of the breakdown of large agglomerates as they are forced through the die. Alford et al. (1987) demonstrated a direct correlation between measured process flaws (measured by microscopy of polished alumina surfaces) and extrudate strengths (obtained from three-point bending tests). They associated these flaws with the presence of powder agglomerates. It is therefore desirable to detect the presence of agglomerates in the paste and make corrective changes to the process to ensure an extrudate of acceptable quality.

The correlation between agglomerate breakdown and spikes in the pressure signal was originally reported by Böhm and Blackburn (1994), who observed sharp peaks in extrusion pressure profiles when extruding pastes known to contain agglomerates. The die diameter and entry angle were shown to have an effect on the intensity of these peaks, with smaller diameters and larger angles increasing this intensity, which was also found to decrease when the paste was passed repeatedly through small orifices. This breakage of agglomerates was confirmed by image analysis. The peaks observed are therefore postulated to correspond to agglomerate breakage events.

Retrospective Outlier Analysis

Amarasinghe (1998) classified an outlier as a datum that varies from the mean extrusion pressure by more than 5% of the mean, which was based on the amount of variation encountered in a normal pressure signal for a series of ceramic pastes. He also observed that pits occur over a short period, and featured large magnitudes. His outlier detection technique was based on a differenced signal:

$$y_t = x_{t+1} - x_t \tag{1}$$

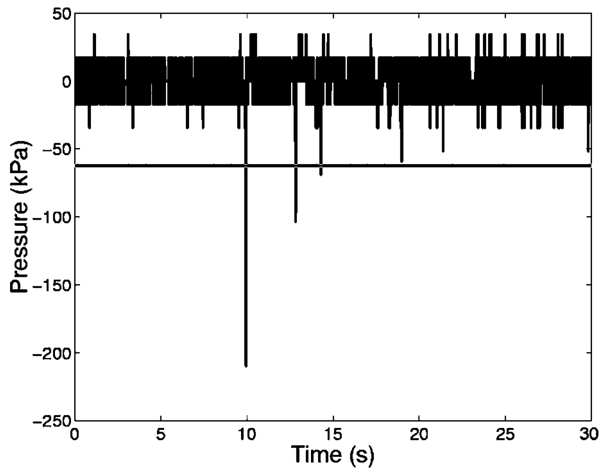
where y_t is the differenced signal and x_t is the original signal. The number of points below the cutoff point corresponds to the number of pits in the pressure signal. This is illustrated in Figure 2(a), which plots the differenced signal along with the cutoff value (grey line) and yields three pit events. The original signal in Figure 2(b) shows that there may have been several more pits and highlights the shortcoming in this threshold approach, although it is very fast.

Moreover, threshold analysis is suitable only for low sampling frequencies, due to the criterion that the pits in the pressure signal must occur rapidly. If too many data points are recorded during a single pit event, which arises at the high sampling frequencies required for fast extrusion, then the differenced signal does not detect an outlier. The other drawback of this method for outlier detection is the assignation of the threshold value; the pit magnitude, particularly in the differenced signal, may not always be greater than the set fraction (here, 5%) of the mean pressure. It is therefore desirable to use a more objective criterion for outlier detection.

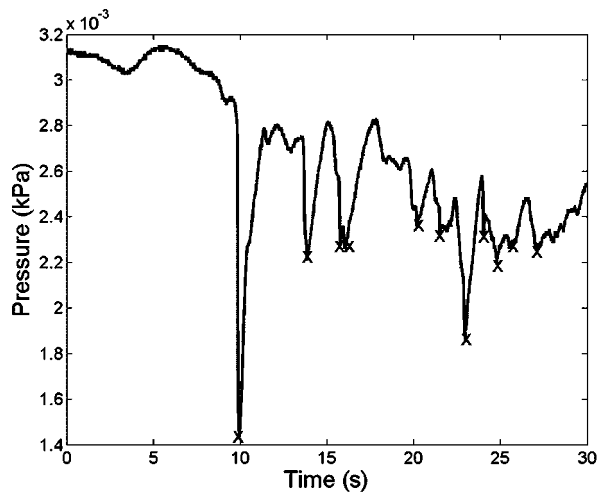
Bayesian methods represent a more rigorous mathematical technique for detecting outliers: these quantify how observations of an event in the past affect its chance, or probability, in the future. In this approach the pressure signal is modeled as a series of data points, d_i, of series length N and overall mean value μ_1, corrupted by Gaussian noise. Gaussian noise is used in the absence of information supporting another form. An outlier, of value μ_2, is hypothesized to occur at some value $i = m_o$ in the data series. This model is then applied over a range of possible values of m_o, and the probability that it is correct, p, is calculated for each m_o. The derivation of this probability can be summarized as (Russell et al., 2003):

$$p(m_o|dI) \propto \frac{1}{\sqrt{N}} \left[\sum_{i=1}^{m_o-1} d_i^2 + \sum_{i=m_o+1}^{N} d_i^2 - \frac{1}{N} \left(\sum_{i=1}^{m_o-1} d_i + \sum_{i=m_o+1}^{N} d_i \right)^2 \right]^{-(N-2/2)} \tag{2}$$

The above approach has been shown to work on ram extrusion data sets and is sufficient for determining the presence of outliers on a retrospective basis. The crosses in Figure 2(b) denote the outliers identified by this method; more outliers are tagged and include those identified by the threshold method. Despite the improvement in objectivity, the Bayesian approach is not as well suited to real-time outlier detection due to the iterative nature of the algorithm, although the calculations are relatively



(a)



(b)

Figure 2. (a) Cut-off method applied to differenced signal, (b) original pressure signal. Conditions: ram extrusion of ceramic paste, $L/D = 48/3$ mm/mm, ram speed $= 1$ mm/s. Crosses: outliers identified by Bayesian method.

fast. More significant, however, is the validity of the assumption that outlier events can be treated as sharp delta functions. At the high sampling rates necessary for real-time analysis in order to remove hardware noise or match the speed of the process, many data points can then be recorded for a single outlier event invalidating the delta approximation, as illustrated in Figure 3.

Real-Time Outlier Analysis

An alternative method of outlier detection is based on gradient analysis, or identification of a continuously increasing or decreasing trend, i.e., the longer the continuously increasing (or decreasing) trend, the greater the likelihood of a spike (or pit).

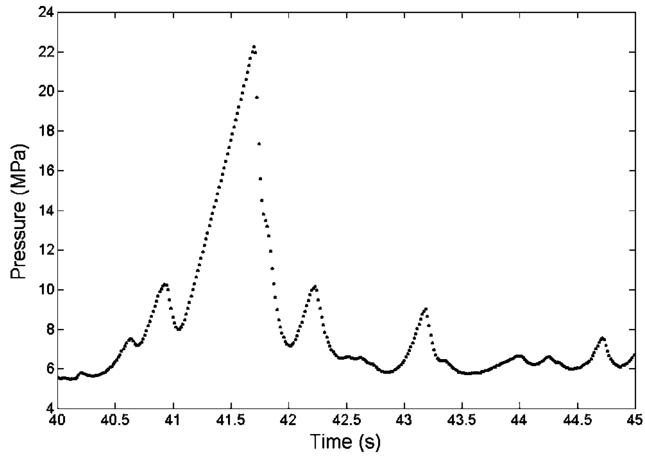


Figure 3. Signal with spike, showing many data points for a single outlier event during extrusion. The spike in this case is an extreme example for the purposes of illustration. Conditions: ram extrusion of ceramic paste, $L/D = 0/1$ mm/mm, ram speed $= 1$ mm/s.

In addition, it has been found that the greater the slope, the greater the probability of it indicating a true outlier. Thus a combination of trend length and gradient, particularly the latter, forms the basis for outlier detection in real time. This is illustrated in Figure 4, which shows marked clustering behavior for normal data and outliers, in this case spikes, during ram extrusion of two different pastes. This trend-based method has been found to be very successful in detecting the presence of outliers in continuous extrusion signals; Figure 5 shows one such example. This technique is ideally suited to real-time analysis, although assignment of the spike or pit threshold still requires some initial trials or benchmarking. In comparisons with the

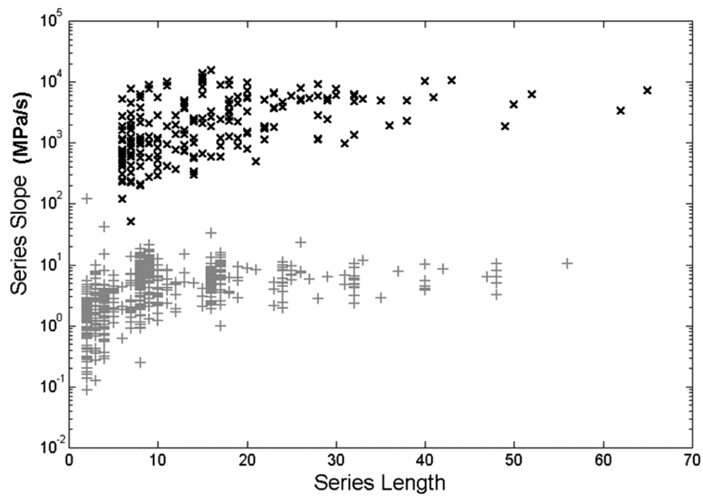


Figure 4. Comparison of series slopes and lengths for spikes (×) and no spikes (+). Conditions: ram extrusion of ceramic and soap pastes, $L/D = 0/1$ mm/mm, ram speed $= 1$ mm/s.

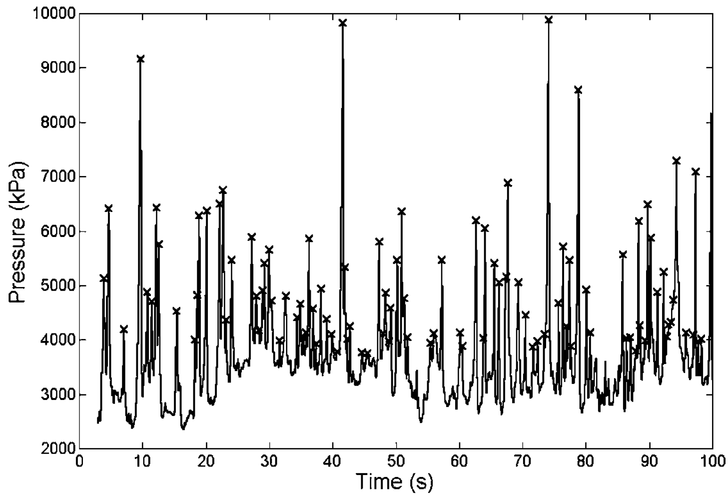


Figure 5. Trend-based method to detect outliers (spikes) in the pressure signal. Conditions: continuous extrusion of ceramic paste, $L/D = 0/1\,\text{mm/mm}$, ram speed $= 1\,\text{mm/s}$. Identified spikes are marked as $\times$.

Bayesian method, this series-based technique proved superior in both real-time applicability and accuracy: it detected outliers more reliably than the Bayesian, while both returned low rates of false negatives.

Analysis of Paste Homogeneity

Maldistribution of the solid and liquid phases in the paste frequently results in a reduction in product quality or extruder performance. Amarasinghe and Wilson (1999) showed that local variation in the pressure signal can be related to particle-particle and particle-fluid interactions and therefore gives an indicator of paste homogeneity. They reported the use of two complementary techniques to quantify this signal noise: standard error analysis and fractal analysis.

Standard Error Analysis

Standard error analysis quantifies the deviation in a data set from an expected trend. For paste extrusion data a moving average is used for the expected trend and the variations are expressed as a percentage of the mean pressure as the coefficient of variation, CV. The key aspect is the selection of the moving average time scales, and Amarasinghe and Wilson proposed the use of a long and a short interval, yielding CV_{global} and CV_{local} respectively, with the period for CV_{local}, N_1 points, being based on an estimate of the time the paste spent in the die, while that for CV_{global}, N_2, was based on the time the paste spent in the barrel. For a given paste, smaller and more uniform pressure fluctuations, i.e., a smooth signal, indicate a more homogeneous paste. The absolute magnitude of the fluctuations (and CV) varies between pastes: Russell et al. (2003) report benchmarking work using ram extrusion to establish normal values of CV (effectively quality set-points) for a well-mixed paste under various extrusion conditions. Experiments on a twin-screw extruder (Russell et al.,

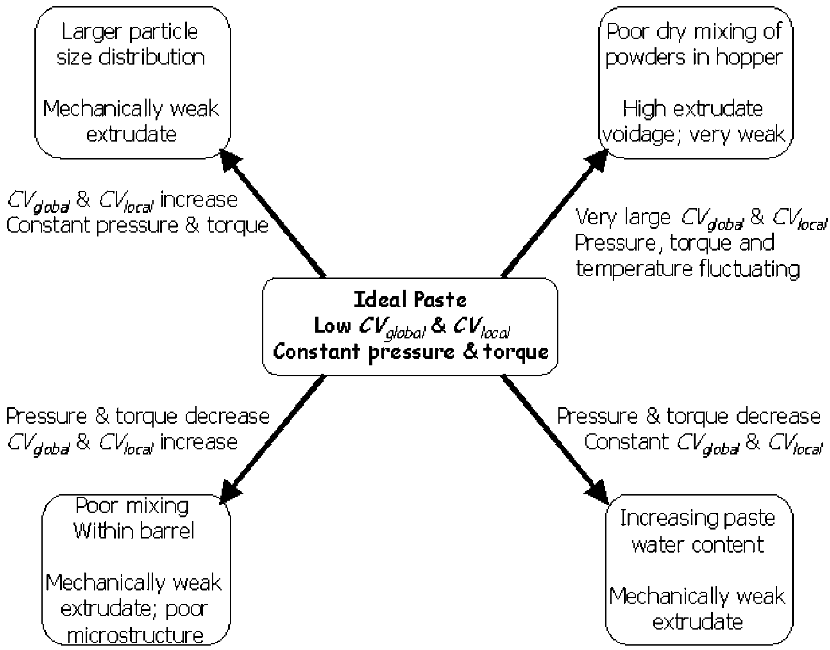


Figure 6. Summary of standard error analysis for screw extrusion of detergent paste.

2004) confirmed that larger pressure fluctuations are associated with a less homogeneous paste. Furthermore, standard error analysis computation is ideally suited to real-time analysis, as the algorithm features continual updating of series.

The two CV values are particularly useful when used in a multivariate framework for quality monitoring in combination with measurements such as mean pressure, torque applied to the screws, and barrel temperature. Figure 6 summarizes the results from screw extrusion of a detergent paste featuring an aqueous liquid phase and a mixture of particulate solids subject to different process and feed disturbances reported by Russell et al. (2004). Increases in CV values from set-points, accompanied by lower pressures and torques, indicate poor mixing of the paste by the action of the screws in the barrel and results in poor mechanical properties of the extrudate. Decreases in the measured values of mean pressure and torque, without change in CV, indicated high paste liquid content, also leading to a mechanically weaker extrudate. Poor mixing of the different powder components prior to feeding resulted in CVs increasing by around an order of magnitude, as well as marked fluctuations in the mean pressure, temperature, and torque. This yields an extrudate with high voidage and very poor mechanical properties. Finally, broader particle size distributions of the powder components resulted in larger CVs, while the mean pressure and torque remained near their set-points–indicating how statistical process control (SPC) methodologies would be insensitive to these microstructural variations.

Figure 6 also suggests that fuzzy logic, Kalman filtering, or neural network techniques could also be applied to such systems, since several different parameters are considered in parallel. However, relatively simple multivariate methods are likely to be adequate here, as these are able to detect and diagnose the system disturbances noted above, while more complex techniques would have limited extra benefit.

Fractal Analysis

Fractal analysis is a method for quantifying patterns in the data: the Hurst Parameter, H (Hurst, 1951), gives a measure of the overall variation of a signal compared to the variation of a short block of the same signal. Since these fluctuations are related to paste homogeneity, fractal analysis is potentially able to quantify this property. Values of H lie between 0 and 1, with 0.5 indicating Brownian motion; in paste extrusion, an H value of 0.5 is hypothesized to indicate a homogeneous paste where particle-particle and particle-fluid interactions causing pressure fluctuations are perfectly random events. Values of H greater than 0.5 are indicative of an overall smoother signal, while those below 0.5 are from locally noisier signals. A case could therefore be made that, for a physically homogeneous paste, H should lie closer to 1 than 0.5, as this indicates a locally smoother signal. However, it is also possible to obtain high H values for a poorly mixed paste, where the overall noise is much greater than the local noise, and thus the more likely value indicating perfect homogeneity is 0.5. Fractal techniques have been used to characterize three-phase fluidized beds (Kwon et al., 1994) and bubble columns (Drahos et al., 1992); Amarasinghe and Wilson (1999) used similar methods, namely Hurst's rescaled range analysis, RRA (Hurst, 1951), to characterize paste ram extrusion pressure data retrospectively. Fractal analysis offers enhanced definition over standard error analysis, and the following sections evaluate several methods for estimating H that could be applied to paste extrusion data. The methods were assessed and compared using artificial data series, generated numerically to reproduce specified values of H, before comparison with experimental data collected from extrusion of a detergent paste.

Test Data

Artificial data sets were generated using a modified form of the algorithm reported by Makse et al. (1996). Firstly, a random signal, x, of length N is generated. This was chosen from a normal distribution with mean zero and variance one, using Matlab's (Version 5.3.1, Mathworks, Inc.) random number generator *randn.m*. This random sequence is then transformed into the frequency domain using the Fourier transform to produce the random signal x_f. It has been established previously (e.g., Heneghan and McDarby, 2000) that fractal properties, including the Hurst parameter, are related to the rate of spectral decay. The relationship between spectral density and frequency can be described as:

$$\Phi \propto \frac{1}{\omega^{\alpha_D}} \tag{3}$$

where Φ is the spectral density, ω is the frequency, and α_D is termed the spectral decay exponent, expressing the rate of spectral decay. The relationship between α_D and H is straightforward, the exact relationship depending on whether the data contain fractional Gaussian noise (*fGn*) or fractional Brownian motion (*fBm*), with the latter applying to these data sets (Cannon et al., 1997). For *fGn* the correlation among its random variables is specified by Equation (4) relating the lag n autocorrelation coefficient ρ_n to the Hurst parameter.

$$\rho_n = \left(|n+1|^{2H} - 2|n|^{2H} + |n-1|^{2H}\right) \tag{4}$$

Cumulative sums of *fGn* are defined as fractional Brownian motion. The relationship between α_D and H is

$$\alpha_D = 2H + 1 \tag{5}$$

Specifying the value of α_D in Equation (3) determines the value of H for a generated signal in the frequency domain, $x_{f\alpha}$: the signal was finally transformed into the time domain to give an artificial signal with known predetermined characteristics, x_H, and fractal characteristics of the data sets extracted using the different techniques.

Rescaled Range Analysis (RRA). This is the method developed by Hurst (1951), and used by Kwon et al. (1994). The discrete, random record, $X(t)$, is divided into a set of subrecords of equal length, δ (referred to as the lag). The mean value within a sub-record from $T = t+1$ to $T = t+\delta$ can be written as:

$$mean = \left(\frac{1}{\delta}\right)[X^*(t+\delta) - X^*(t)] \tag{6}$$

$$X^*(t) = \sum_{u=1}^{t} X(u) \tag{7}$$

where $C(t,u)$ is the cumulative departure of $X(t+u)$ from the mean of the sub-record:

$$C(t,u) = [X^*(t+u) - X^*(t)] - \left(\frac{u}{\delta}\right)[X^*(t+\delta) - X^*(t)] \tag{8}$$

The sample sequential range, $R(t,\delta)$, is defined as:

$$R(t,\delta) = \max_{0\le u\le\delta} C(t,u) - \min_{0\le u\le\delta} C(t,u) \tag{9}$$

The sample sequential variance of the sub-record S_H^2 is given by:

$$S_H^2(t,\delta) = \left(\frac{1}{\delta}\right)\sum_{u=t+1}^{t+\delta} X^2(u) - \left[\left(\frac{1}{\delta}\right)\sum_{u=t+1}^{t+\delta} X(u)\right]^2 \tag{10}$$

For each sub-record, the standard deviation, S_H, and the cumulative range, R, are calculated. The average of all the sub-records gives the final value for R/S_H for the given time lag. A series of R/S_H values can be obtained as a function of the lag; $\delta : R/S_H$ is termed the rescaled range and has the scaling property:

$$\frac{R(\delta)}{S_H} \propto \delta^H \tag{11}$$

where H is the Hurst parameter. Figure 7(a) illustrates a typical signal displaying fractal characteristics, using the algorithm generated by Makse et al. (1996) for an H value of 0.5. Such a signal was used to determine the most suitable fractal analysis methods in the following discussion. Figure 7(b) is a typical plot for estimating H using RRA applied to the artificially generated data set shown in Figure 7(a).

Detrended Fluctuation Analysis. A popular alternative estimator of fractal properties to RRA is detrended fluctuation analysis (DFA) (Heneghan and

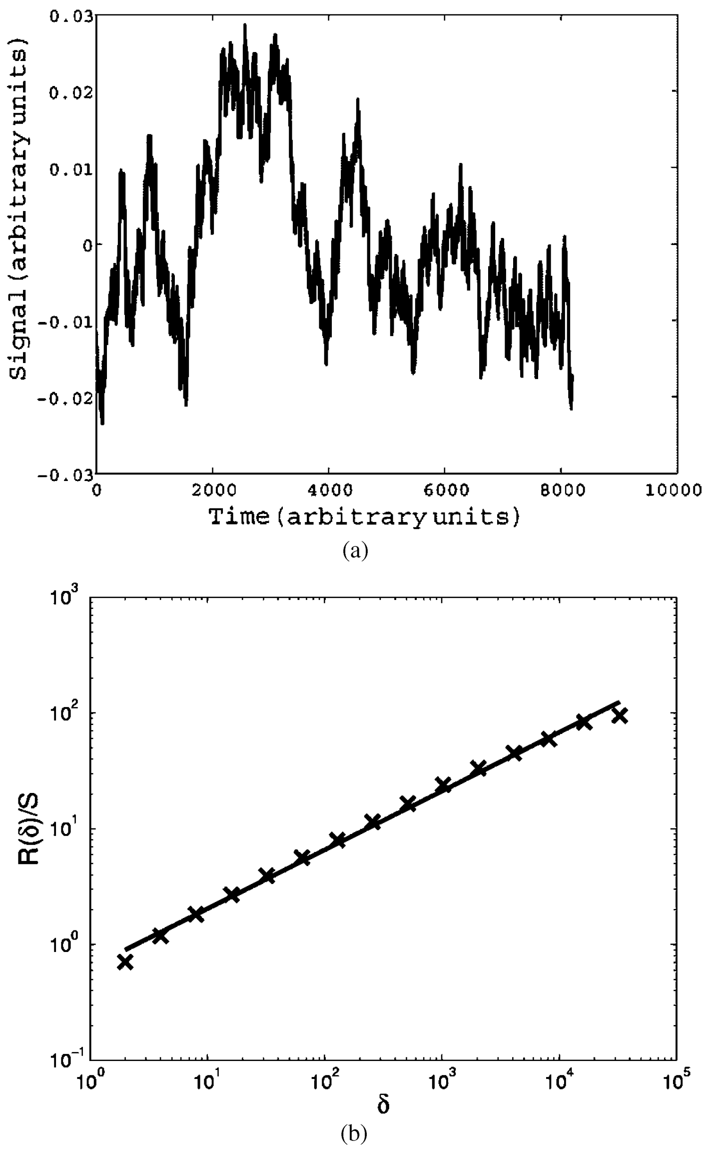


Figure 7. (a) Example of random signal (fractional Brownian motion) generated using the algorithm reported by Makse et al. (1996) for $H = 0.5$, (b) example of RRA for estimating H: log-log plot of R/S_H versus δ, for the data in (a), the gradient of which yields H.

McDarby, 2000). A running summation sequence is generated for the discrete, random record $X(t)$:

$$y(n) = \sum_{t=1}^{N-1} X(t)$$

$$\begin{aligned} y(0) &= 0 \\ y(N) &= 0 \end{aligned} \tag{12}$$

where N is the length of the series. The entire sequence is divided into M nonoverlapping blocks, $y_m(N)$, each containing K samples of block length L_B:

$$y_m(n) = y(mK + N) \tag{13}$$

with the following limits:

$$\begin{aligned} 0 \le m \le M - 1 \\ 0 \le N \le K - 1 \end{aligned} \tag{14}$$

The local trend in each block is defined to be a linear, least-squares fit to the samples in that block. The trend is denoted as $y_{m,t}(N)$. A detrended signal is defined for each block as the difference between the original signal and the local trend for that block:

$$y_{m,d}(N) = y_{m,t}(N) - y_m(N) \tag{15}$$

The variance of the detrended signal is calculated for each block. $F(K)$ is then defined as the average of the variances over all the blocks:

$$F(K) = \left(\frac{1}{M}\right) \sum_{m=0}^{M-1} \mathrm{var}(y_{m,d}(N)) \tag{16}$$

It has been shown (e.g., Buldyrev et al., 1995) that $F(K)$ exhibits power law dependency on K:

$$F(K) = K^{\beta_D} \tag{17}$$

where β_D is simply $\alpha_D + 1$, which can in turn be related to H as discussed previously. Figure 8 illustrates the determination of H using DFA.

Moving Average Analysis (MAA). Vandewalle and Ausloos (1998) argued that H could be estimated by looking at the density ρ_m of crossing points between any two moving averages. The algorithm involves generation of two moving averages

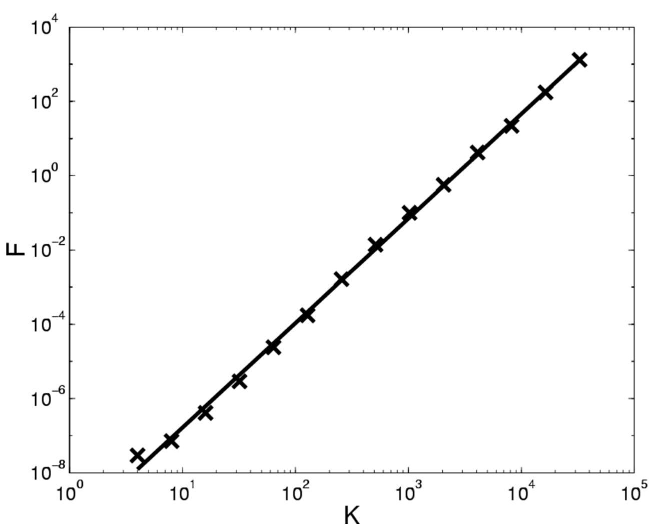


Figure 8. Example of relationship between average block variance (F) and number of samples (K) involved with detrended fluctuation analysis for estimating H. Signal processing applied to data sets generated artificially using the technique reported by Makse et al. (1996).

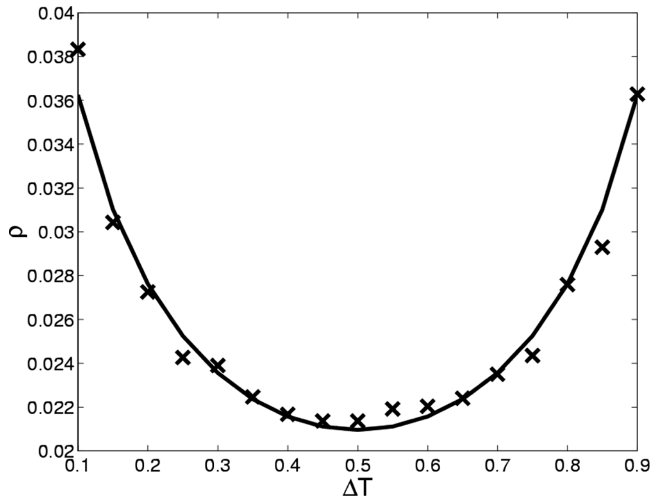


Figure 9. Example of relationship between ΔT and ρ_m obtained during moving average analysis for estimating H. Signal processing applied to data sets generated artificially using the technique reported by Makse et al. (1996).

from the original signal. The period of the first moving average, T_2, is an arbitrary function of the total signal length; the period of the second moving average, T_1, is a function of T_2. The relative difference between these periods, ΔT, is defined as:

$$\Delta T = \frac{T_2 - T_1}{T_2} \tag{18}$$

The number of times these moving averages crossed can then be related to H:

$$\rho_m \propto \frac{1}{T_2}[(\Delta T)(1 - \Delta T)]^{H-1} \tag{19}$$

T_2 was chosen to collect data sampled over 0.5 s (approximately 125 sample points), although it should be noted that the value was arbitrary and Equation (19) indicates that absolute values are accounted for with ΔT; practically, the value of T_2 will determine the resolution of the analysis. The variation of ρ_m is shown in Figure 9.

Spectral Decay Exponent (SDE). This method is related to the method for generating the artificial signals, i.e., measuring the rate of spectral decay of the data in the frequency domain. This gives a value for α_D that in turn is related to H through Equation (5).

Comparison of Fractal Analysis Methods

The methods are reviewed in terms of data points required for a reliable estimate of H, sensitivity to various overall trends in the data, and suitability for real-time fractal analysis.

Both RRA and DFA were found to require at least 2^{15} data points in order to estimate the Hurst parameter of the artificial signals with 95% confidence; this is consistent with the conclusions reported previously (Cannon et al., 1997). The typical length of data series collected in our ram extrusion experiments was less than half this value, rendering both these methods unsuitable. One solution is to increase the sampling frequency to ensure that enough data points are recorded to give sufficient accuracy. However, in our experience the process and material related fluctuations usually do not occur at rates above 100 Hz, so that increasing the sampling rate would only add pressure transducer noise to the signal, which in turn requires de-noising. Furthermore, both RRA and DFA were found to be very sensitive to sinusoidal components in the data, reducing their suitability for auger machines. Hu et al. (2001) have demonstrated that it is possible to obtain an estimate of H from data corrupted with sinusoidal signals (with the DFA technique), although this method may not necessarily work with paste extrusion data.

MAA required at least 2^{17} data points to give the desired confidence levels, so was deemed insufficiently accurate for these applications. MAA is not, however, as sensitive to sinusoidal components and is also easily adapted to real-time analysis.

SDE fared best in terms of accuracy (2^8 data points required for 95% confidence) as well as resilience to sinusoidal components. It is, however, affected by transducer noise, which had to be removed before its application. Russell et al. (submitted) discuss this type of de-noising in more detail: it essentially involves splitting the signal into high-frequency components and low-frequency components. The transducer noise dominates the high-frequency components, and this is dealt with before recombining the high and low frequencies into the de-noised signal. The retrospective SDE method, based on conventional Fourier methods, is unsuitable to real-time analysis due to its poor time resolution. However, a similar method of estimating the spectral exponent has been developed by Abry and Veitch (1999), using wavelet analysis instead of Fourier analysis. Wavelets are ideally suited to real-time analysis, and the relationship between α_D and H remains the same. Full details of the AV estimator can be found in the original article. This method was applied to the screw extrusion results discussed in the next section.

Results from Fractal Analysis

Applying the SDE method to data from approximately 250 ram extrusion experiments showed that the extent of mixing affects H as well as the CV values. Data were taken primarily from experiments using detergent paste, which featured varying amounts of mixing. The results showed that the better the paste was mixed, the lower the CV values and the closer H approximated the ideal value of 0.5.

Thus a multivariate analysis, such as that presented by Russell et al. (2003), can be very useful in investigating the effect of mixing on paste homogeneity. Apart from this case, the majority of extrusion parameters such as die geometry and extrusion rate showed little effect on either H or CV, indicating that these did not affect paste homogeneity, which was expected for these simple die systems.

Fractal analysis was, however, found to suffer from a general lack of sensitivity compared to results from standard error analysis. The major reason for this lack of sensitivity is that H can vary only from 0 to 1, so that major changes in paste homogeneity would not result in a large absolute change in the value of H. Standard error analysis does not suffer from this limitation; it is a semi-infinite parameter in theory as the values can exceed 100%. This is illustrated in Figure 10, which shows H and CV_{global} obtained from screw extrusion tests where the homogeneity of the paste was disrupted by the addition of pre-compacted material. The standard error analysis parameter shows a large variation, while H is clustered around the "ideal" value of 0.5 and little can be deduced from this measurement. The 68% confidence interval ellipse shows that the major axis lies on the CV_{global} axis.

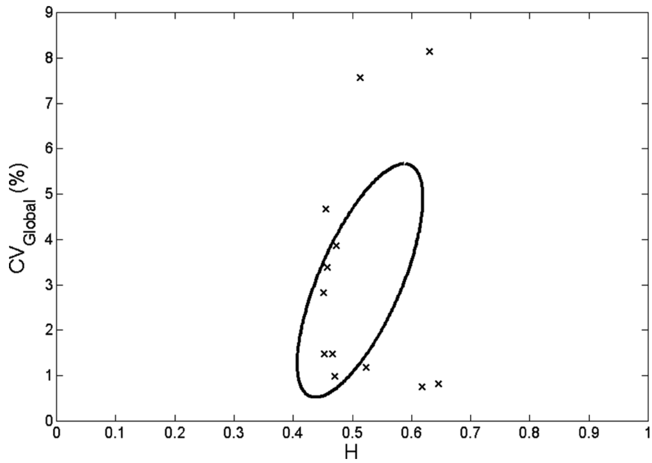


Figure 10. Comparison of H and CV_{global} for data obtained from screw extrusion of detergent pastes where homogeneity varied due to deliberate addition of compacted material. Conditions: $L/D = 6/1$ mm/mm, speed = 200 rpm, $T_D = 40$°C. Ellipse shows 68% confidence interval.

In the one case where H exhibited a significant systematic variation, namely for differences in dry powder mixing, the CV values increased by an order of magnitude (Russell et al., 2004). The information provided by fractal analysis was therefore redundant, as less sophisticated techniques were capable of detecting this attribute. The application of fractal analysis to these systems, particularly in a real-time context, is therefore limited.

Spectral Analysis

The generation of surface fractures represents a major challenge in paste extrusion as these compromise the mechanical properties of the extrudate as well as being aesthetically unacceptable (Abry and Veitch, 1999). Figure 11 shows an example of circumferential fracture and indicates that this type of defect is periodic in nature.

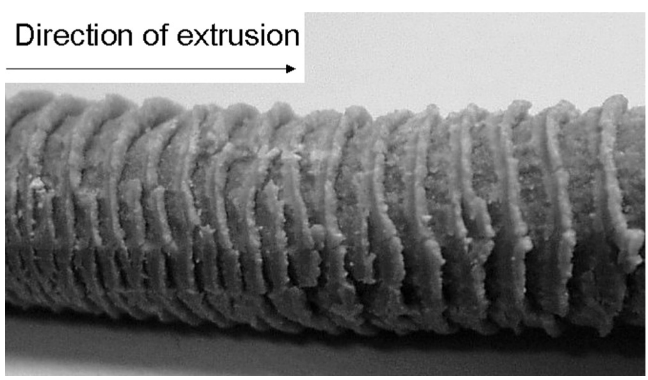


Figure 11. Example of circumferential surface fracture of paste extrudate generated during ram extrusion. Conditions: detergent paste, $L/D = 0/9$ mm/mm, ram speed = 1 mm/s.

Amarasinghe and Wilson (1998) demonstrated that such fracture is accompanied by periodic components in the extrusion pressure, which could be isolated by Fourier analysis and exhibited the same frequency as that seen in visual observations. Domanti and Bridgwater (2000) reported that circumferential fracture often features a periodicity corresponding to half the die diameter, yielding a simple prediction of the fracture frequency for a given extrusion geometry: this frequency is here termed the Domanti frequency. The power spectrum presented in Figure 12 is based on data taken from an experiment where the starch dough extrudate displayed fracture at approximately 31 Hz; the peak observed in the frequency domain lies very close to this frequency. Detection of significant periodic components at this frequency can therefore be related to the occurrence of fracture: in all tests with three pastes, false positives for this rule were not observed. False negatives were occasionally recorded, mainly at low speeds where the Domanti frequency lay within the low-frequency band where the signal-to-noise ratio is characteristically poor. The mechanism of fracture in pastes is not fully understood, although recent work has shown that wall shear stress in the die land plays an important role (Kulikov and Hornung, 2001).

As with fractal analysis, Fourier methods are poorly suited to real-time spectral analysis. Wavelets were considered as an alternative to Fourier-based spectral analysis, but while their resolution in the time domain is excellent, and the algorithm ideally suited to real-time implementation, the frequency domain resolution was somewhat limited, and this has been shown to be the case in other systems (e.g., Daubechies, 1992).

A Bayesian approach to spectral analysis has been adopted and proved effective, both in terms of real-time applicability and in sensitivity to periodic components (Bretthorst, 1989). This is again a model-based approach: here the pressure signal is modeled as a sinusoidal signal of a single frequency, ω, corrupted by Gaussian noise:

$$f(t) = A\cos(\omega t) + B\sin(\omega t) \tag{20}$$

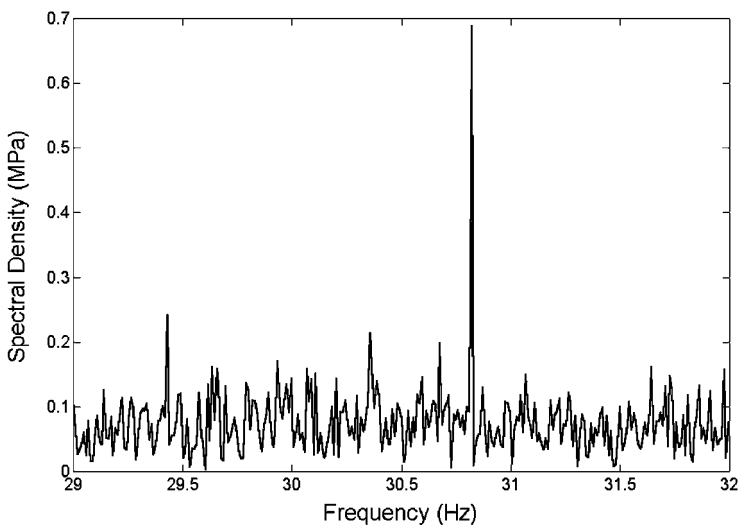


Figure 12. Spectral analysis of pressure data for which paste exhibited fracture at approximately 31 Hz. Conditions: $L/D = 0/4$ mm/mm, ram speed = 1 mm/s, ram extrusion of starch dough.

This system has been investigated extensively by Bretthorst (1989) and further developed by Ó Ruanaidh and Fitzgerald (1996). The probability of ω given the data can be shown to be:

$$p(\omega|dI) \propto \left[1 - \frac{2E(\omega)}{\sum_{i=1}^{N} d_i^2}\right]^{2-N/2} \tag{21}$$

where, as before, N is the length of the data series d. $E(\omega)$ can be defined as:

$$E(\omega) = \frac{1}{N}(G^2(\omega) + Q^2(\omega)) \tag{22}$$

with $G(\omega)$ and $Q(\omega)$ defined thus:

$$G(\omega) = \left(\sum_{i=1}^{N} d_i \cos(\omega t)\right) \tag{23}$$

$$Q(\omega) = \left(\sum_{i=1}^{N} d_i \sin(\omega t)\right) \tag{24}$$

The probability expressed in Equation (21) approaches its maximum value if most of the data energy is concentrated around a single frequency, ω. Ó Ruanaidh and Fitzgerald have shown that this approach is very good at detecting the presence of a single sinusoidal signal in the presence of noise. For paste extrusion applications, it is also necessary to estimate the amplitude of the signal in the time domain. A simple least-squares technique, as outlined by Stoica et al. (2000), was used. The Bayesian method requires only approximately 150 data points for an effective estimation of the presence of a sinusoidal signal, and since sampling rates are often in the order of 100 Hz, this represents a new estimation every 1.5 s or so, making it a reasonably good real-time measurement. Since the Domanti frequency can usually be calculated for a given geometry and extrusion rate it would then be possible to monitor its amplitude, and if this approaches the fracture threshold, then appropriate action could be taken to suppress the predicted surface fracture. At this stage, however, the form of appropriate control action is not clearly understood, as most fracture solutions feature geometrical methods or hardware modifications.

Comparison

The need to establish benchmarks for each material is illustrated by Figure 13, which shows the variation in CV_{local}, a homogeneity indicator, as the die length was varied. Similar plots for other process parameters are given by Russell (2004). It can be seen that the starch paste features the lowest value of CV_{local}, which can be related to its formulation (soft particles and viscous liquid matrix). The ceramic paste, with hard particles and water entrapped in capillaries and micro-voids, presents the noisiest signal, while the detergent paste lies in between. Values for the detergent paste at die lengths longer than 12 mm are not plotted as the work requirement for extrusion was too high for the process equipment. The different materials therefore give noticeably different quantitative responses to similar variations in process conditions. Application to different materials will most likely require some independent

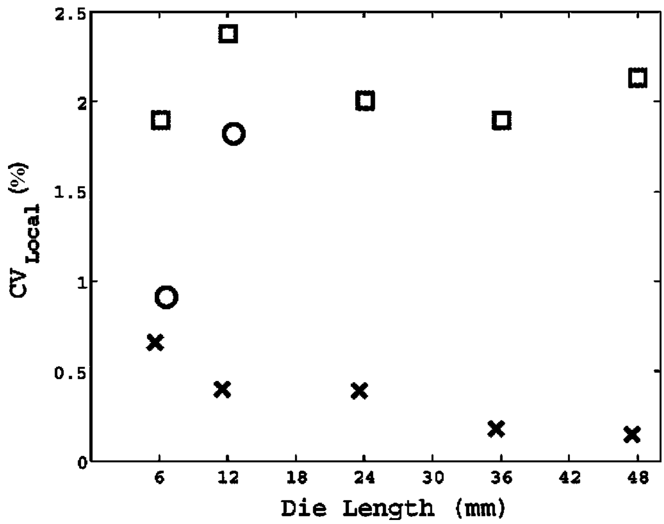


Figure 13. Effect of die land length on CV_{local}. Crosses: starch; squares: ceramic; circles: detergent. Conditions: ram extrusion, $D = 3\,\text{mm}$, ram speed $= 1\,\text{mm/s}$.

microstructural analysis in order to relate the quantified fluctuation trends to physical interpretations, such as extent of fat melting in chocolate extrusion (Russell et al., 2005).

Conclusions

Retrospective signal processing techniques, initially developed with ram extrusion, have been successfully extended to continuous screw extrusion data and can be implemented in real-time. These monitoring methods also have potential for development of on-line control of paste extrusion processes.

A Bayesian-based outlier detector was shown to be the most mathematically rigorous method of identifying outliers in the signal, corresponding to the bursting of pockets of entrapped air or the breakdown of large agglomerates. However, it failed to detect outliers if many data points were sampled for a single outlier event. A gradient-based outlier detector has been developed, and this proved to be the most robust method for detecting outliers, as well as being ideally suited to real-time analysis.

The signal noise level is ultimately related to the paste homogeneity. Of the two techniques presented for quantifying signal noise, standard error analysis was found to give more specific information related to paste quality, particularly in the multivariate space, than fractal analysis. The increased computational complexity in fractal analysis methods without marked improvement in sensitivity also reduced their attractiveness.

A Bayesian sinusoidal signal estimator has been shown to have good potential for real-time spectral analysis of pressure signals.

Application to experimental data has highlighted the need to perform benchmarking tests in order to map the fluctuation quantifiers to physical phenomena.

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Nomenclature

A	trivial sinusoidal amplitude
B	trivial sinusoidal amplitude
C	cumulative departure
CV	coefficient of variation, %
CV_{global}	global coefficient of variation, %
CV_{local}	local coefficient of variation, %
d_{i}	data series for Bayesian model
D	die diameter, mm
E	term in Bayesian spectral estimator
$f(t)$	signal in time domain, Pa
F	average variance of detrended signals
G	term in Bayesian spectral estimator
H	Hurst parameter
i	point in data series
I	a priori information for Bayesian model
K	number of samples per block
L	die land length, mm
L_{B}	block length
m	point within block
m_o	point at which outlier occurs
M	number of nonoverlapping blocks
n	lag
N	length of data series
N_1	length of mean for local CV
N_2	length of mean for global CV
p	probability
Q	term in Bayesian spectral estimator
R	sample sequential range, Pa
S	sample sequential variance
S_H	standard deviation of sub-record
t	time, s
T	time within sub-record, s
T_D	die temperature, °C
T_1	period of moving average, s
T_2	period of moving average, s
u	point within sub-record
x_i	random signal in time domain
X	random record, Pa
X^*	mean value of sub-record, Pa

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