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ROUTINE ANALYSIS OF MOLASSES AND MIXED JUICE BY NIR SPECTROSCOPY

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Abstract

A Bruker Near Infra-red Spectrometer (NIRS) was purchased by the Sugar Milling Research Institute for the weekly analysis of mixed juice and final molasses for the 2007-2008 season. The NIRS system was set up for high sample throughput requiring minimal analysis time. Samples were simultaneously tested by traditional laboratory methods as well as by NIRS, allowing week-by-week analysis of the NIRS predictive capabilities.

Mixed juice comparisons were made for pol, Brix, conductivity ash, fructose, glucose and sucrose. The NIRS predictions showed excellent precision, comparable to the laboratory method tolerances. Molasses comparisons were made for pol, Brix, dry solids, conductivity ash, fructose, glucose, sucrose and a target purity difference (TPD) calculated from the NIRS predictions. A 'Hybrid TPD' using a combination of laboratory and NIRS generated results was also monitored. For molasses samples the predictions showed improvement over previously published data. Weekly differences between laboratory and NIRS results were monitored for each analyte for each factory, and were also pooled to create a season summary.

Keywords: analysis, calibrations, comparison, mixed juice, molasses, NIRS, quality control

Introduction

The major advantage of using Near Infra-red Spectroscopy (NIRS) is the short analysis time required to obtain results for many sample properties and components. The skills needed by a NIRS operator in the quality control environment are minor compared with skills required to produce the same results using the variety of laboratory test methods. In the factory environment, testing skills are frequently lost through staff promotion or loss, with the possible lowering of laboratory standards.

Testing by NIRS requires only simple sample preparation for molasses and none for mixed juice (MJ), allowing good results to be obtained, even by relatively inexperienced testers. A further advantage is the ability to estimate properties that otherwise requires considerable skill, time, and equipment. Properly developed NIRS calibration equations should allow molasses pol, Brix, dry solids, ash, sucrose, fructose, glucose and Target Purity Difference (TPD) to be predicted with a simple sample dilution. MJ samples require no sample preparation at all, and a NIRS analysis estimates pol, Brix, sucrose, fructose, glucose and ash content. The use of NIRS testing in the factory environment is therefore a very attractive option.

NIRS calibrations are created by statistical correlation of NIRS spectra of samples with the values determined by the laboratory methods (the reference methods). These calibrations must be robust enough to account for different sample compositions caused by geographical, seasonal, varietal and operational effects. For this reason the NIRS spectra and laboratory results must be correlated for a large number of samples obtained under a wide variety of conditions. Previous work at the Sugar Milling Research Institute (SMRI) focused on the overall predictive capability of the NIRS technique (Schäffler, 2001). The large number of samples correlated during a season can present very good overall correlations, but swamp the performance of the smaller groups of data they comprise. While the previous study broke the overall correlations down to a week-by-week basis, it did not consider the effect of using NIRS predictions on individual factory performance data. This study therefore focused on the performance of NIRS in relation to each sugar factory over the course of the season.

Experimental

Instrumentation

The NIRS system is comprised of a Bruker Multi-purpose Analyser (MPA) fitted with a Metrohm 838 autosampler. No temperature control unit was attached to the MPA; however, the NIRS laboratory was maintained at 20°C by air-conditioning at all times. All spectra were obtained in absorbance mode in the scanning range 800 to 2500 nm using a Hellma flow-through sample cell with a path length of 1 mm. The NIRS software used for spectral processing and calibration creation was OPUS Version 6. This included Opus Lab, which provided a simple interface with mouse-click operation for controlling automated NIRS analysis. This interface was used throughout the season for sample analysis. The initial calibrations used were those developed using a Bruker MPA on loan to the SMRI during 2006 (Schäffler, 2007). Previous studies used instrumentation that required calibration modification when a major component such as a source lamp was replaced (Schäffler, 2005). The source lamp on the MPA used in this study was replaced without the need for re-establishing the calibration.

Handling of mixed juice samples

All MJ samples submitted to the SMRI for weekly analysis were analysed by NIRS. This comprised 19 South African and three African samples each week. Samples were taken according to the prescribed procedure (Anon, 2005: Section 4.1) and composited into weekly representative samples at the SMRI laboratory maintained at 20°C. The composite samples were immediately clarified and filtered for pol and Brix analyses. Portions were kept for the conductivity ash analysis, and for the gas chromatography (GC) analysis for fructose, glucose and sucrose. In addition, an unfiltered portion of the composite was submitted to the NIRS laboratory where it was tested within two hours of initial thawing. Each sample was poured into two vials and a NIRS spectrum for each obtained using Opus Lab. The predicted results from the two spectra were averaged to give the final predicted NIRS results. All laboratory results were generated using the Official Methods (Anon, 2005). Polartronic measurements were made using the wavelength 589nm and lead clarification (Anon, 2005: Method 1.7). Brix was measured by refractometry (Anon, 2005: Method 1.8). Ash was measured by the conductivity ash method (Anon, 2005: Method 3.6). Fructose, glucose and sucrose were determined by gas chromatography (silylation-only) method (Anon, 2005: Method 1.9).

Handling and analysis of final molasses samples

All final molasses samples submitted to the SMRI for routine weekly analysis were analysed by NIRS. This comprised 25 composite samples from South African and other African sugar factories. Samples as received were homogenised and sub-sampled. A single sub-sample was used for all laboratory test methods and the NIRS sample preparation. Each sample was diluted at 16 grams to 100 ml. Each prepared sample was poured into two vials and a NIRS spectrum was obtained for each. The predicted results from the two spectra were averaged to give the final predicted NIRS results. A quality control procedure was set up using three molasses samples of established composition with each batch of samples tested (personal communication[1]). These were used to monitor the NIRS performance on a weekly basis. All laboratory results were generated using SASTA approved test methods (Anon, 2005). Polartronic measurements were made using the wavelength 589nm and lead clarification (Anon, 2005: Method 6.1). Brix was measured by refractometry in all cases (Anon, 2005: Method 6.1). Ash was measured by the conductivity ash method (Anon, 2005: Method 6.4). Dry solids results were determined by the Karl Fischer method (Anon, 2005: Method 6.3), with the exception of four very high dry solids UK[2] samples where the vacuum oven dry solids method (Anon, 2005: Method 6.2) was used. Fructose, glucose and sucrose were determined by high performance anion exchange chromatography (Anon, 2005: Method 6.6).

Calibrations

All seasons and week numbers refer to the South African Sugar Association (SASA) calendar. Calibrations developed by the SMRI using samples from the 2006-2007 season formed the starting point for the 2007-2008 season NIRS analyses. These spectra were obtained using an MPA on loan from the supplier during the latter part of 2006. The SMRI purchased and installed their own NIRS during week 13 of the 2007-2008 season. Spectra obtained from weeks 13 to 23 were added to the calibrations to further improve their robustness towards different sample compositions, and re-optimised. Data presented here thus exclude predictions for samples up to week 22. To improve robustness still further, all spectra were added to the calibration after they had been used to predict the weekly results. For example, when analysing week 30 samples, the calibration included all spectra up to week 29. When the predictions had been made, the spectra from week 30 were then added to the calibration in readiness for week 31 testing. This continued until the end of the season to maximise the calibration robustness to seasonal variation.

Calculations

TPD is calculated using the results for glucose, fructose, sucrose, dry solids and ash using the formula (Smith, 1995):

$$TPD = \frac{sucrose}{drysolids} - [43.1 - 17.5 \times \{1 - e^{-0.74(\text{fructose+glucose})/ash}\}]$$

The Hybrid TPD uses the same formula but uses NIRS ash and NIRS dry solids results, and laboratory-determined fructose, glucose and sucrose results.

Calculations for bias and standard error of prediction (SEP) were taken from Williams (2007).

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[1]Schäffler KJ (2007). Action items for the implementation of NIR for weekly molasses analysis. SMRI internal memorandum.

[2]Sugar factories mentioned in this paper are: (South Africa) AK=Amatikulu, DL=Darnall, ES=Eston, FX=Felixton, GH=Gledhow, KM=Komati, ML=Malalane, MS=Maidstone, NB=Noodsberg, PG=Pongola, SZ=Sezela, UC=UCL Co Ltd, UF=Umfolozi, UK=Umzimkulu; (Malawi) DW=Dwangwa, NH=Nchalo; (Mozambique) MA=Maragra; (Swaziland) MH=Mhlume, UB=Ubombo, SM=Simunye; (Tanzania) MW=Msolwa, RU=Ruembe.

Results and Discussion

Mixed juice

The results presented in Table 1 show the correlation between laboratory and NIRS results from weeks 23 to 43 for the 2007-2008 season. Individual results were excluded as outliers where they exceeded three times the standard deviation from the mean Lab-NIRS value. Week 23 was excluded entirely for glucose, fructose and ash since the calibrations were not optimised at the time of analysis.

Table 1. Summary of near infra-red spectrometer (NIRS) performance for mixed juice.

Analyte (unit)	Sample count	Outliers removed	SEP (%)	Slope	Bias	RSQ	95% confidence limits (%)	Lab method tolerance (%)
Brix (°Bx)	432	0	0.05	0.99	-0.01	1.00	± 0.11	± 0.05
Pol (°Z)	431	1	0.06	0.99	0.00	1.00	± 0.12	± 0.05
Sucrose (%)	409	23	0.06	0.99	0.00	1.00	± 0.12	± 0.10
Fructose (%)	431	2	0.02	0.97	0.00	0.86	± 0.04	± 0.03
Glucose (%)	409	23	0.02	0.96	0.00	0.86	± 0.05	± 0.03
Conductivity ash (%)	404	29	0.04	0.90	-0.01	0.81	± 0.08	± 0.07

SEP = standard error of prediction, RSQ = correlation coefficient squared

The data from Table 1 are represented graphically in Figures 1 to 3, which illustrate the regression lines, slopes, and 95% certainty limits for the respective property. The NIRS predictive capability for each mixed juice property is summarised for each factory in Appendix 1-6.

Mixed juice Brix, pol and sucrose

The Brix, pol and sucrose data from Table 1 are shown graphically in Figure 1(a-c). This figure illustrates excellent slope, bias and correlation coefficient squared (RSQ) statistics for these three components. Comparing the standard error of prediction (SEP) to the precision of the laboratory method is a measure of the NIRS predictive capability. Here the SEP values of 0.05, 0.06 and 0.06% compare favourably with the laboratory precision of 0.05, 0.05 and 0.10% for Brix, pol and sucrose, respectively. The 95% confidence intervals show that only one in 20 NIRS results differ from the equivalent laboratory-generated results by more than 0.12%.

Individual factories (see Appendix 1-3) showed slopes between 0.96 and 1.01, RSQ values of either 0.99 or 1.00, and bias between -0.07 and +0.04% for Brix. Pol results showed slightly more scatter, with RSQ values from 0.98 to 1.00 and slopes from 0.95 to 1.05. NB and NH showed biases of -0.09 and -0.08% respectively, with this over-prediction for NB also evident in the sucrose statistic of -0.08% bias. All other factories showed excellent sucrose correlations.

Mixed juice glucose and fructose

Table 1 and Figure 2 show very good overall correlation statistics for the glucose and fructose analyses. The low concentration of these components (typically 0.3 to 0.4%) and the proportionally large error in the laboratory results compared with sucrose dictate less precision in the NIRS prediction (an absolute error of 0.03% in a laboratory result of approximately 0.3% for fructose and glucose, compared with a 0.1% absolute error in a laboratory result of approximately 11% for sucrose.) This scatter is shown by the RSQ values of 0.86 for both fructose and glucose.

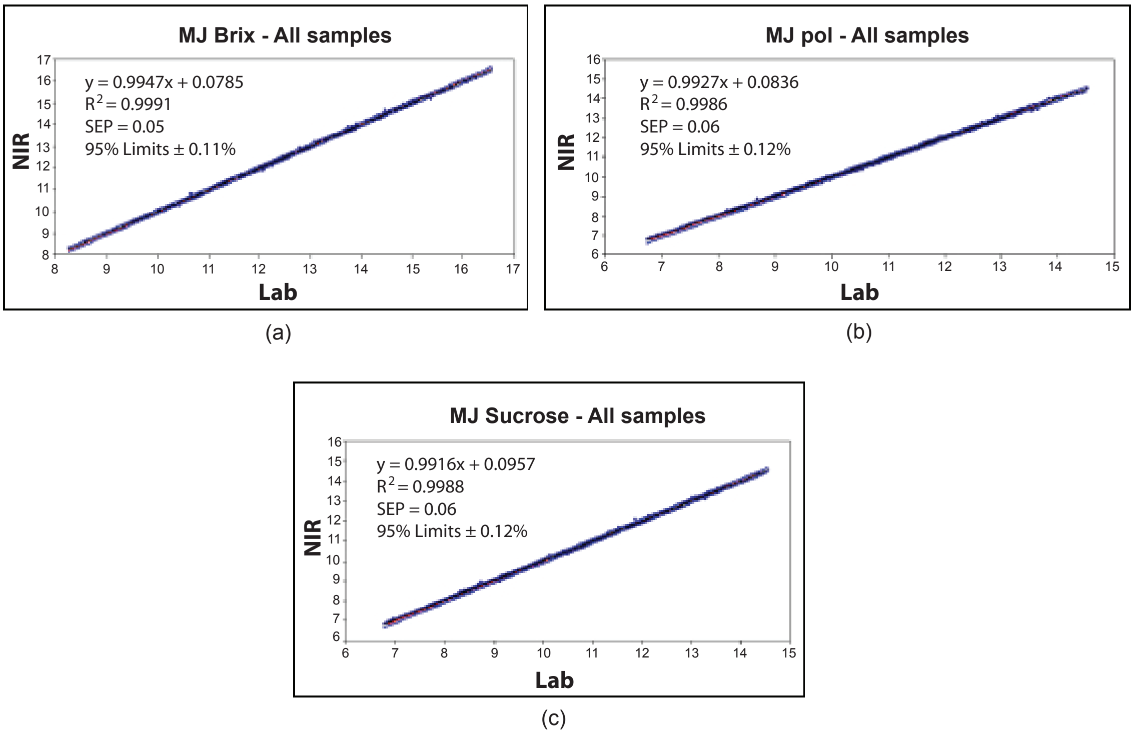
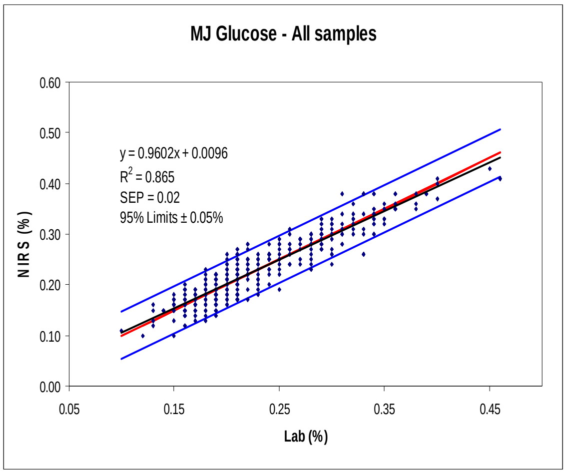
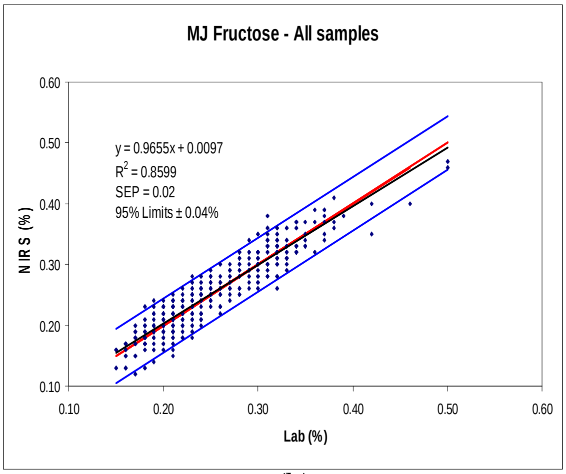


Figure 1(a-c). Scatter plots of near infra-red spectroscopy (NIRS) predictions for mixed juice pol, Brix and sucrose.



(a)



(b)

Figure 2(a-b). Scatter plots of near infra-red spectroscopy (NIRS) predictions for mixed juice glucose and fructose.

None of the factories displayed any evidence of bias in the NIRS results for either glucose or fructose (see Appendix 4 and 5). The confidence limits show that 95% of all NIRS predicted results fall within 0.05% of the laboratory-generated result. SEP values of 0.02% compare well with the laboratory precision of 0.03%. RSQ values for individual factories are poor in comparison with those achieved for sucrose; however, this is attributable to the NIRS precision and the small range of values produced by each factory through the season. MS1, MS2, NB and UC all showed poor slope and RSQ values but no bias. The maximum difference between the laboratory and NIRS values were 0.04% for MS1 and MS2, 0.06% for NB, and 0.06% for UC. All other factories showed differences of less than 0.04%. Similarly MS1, MS2, ES, SZ and UK showed poor correlations for fructose, although again without bias. The maximum differences between the laboratory and NIRS values were 0.04% for MS1 and MS2, 0.05% for ES and SZ, and 0.06% for UK.

Mixed juice conductivity ash

The conductivity ash data from Table 1 is represented graphically in Figure 3. Due to the high purity of MJ and the low concentration of ash, good ash predictions by NIRS would not be expected. Nonetheless, unbiased results with a low SEP of 0.04% were comparable with the laboratory results. The slope of 0.90 and RSQ of 0.81 for all the samples combined show improved precision compared with data reported previously (Schäffler, 2006).

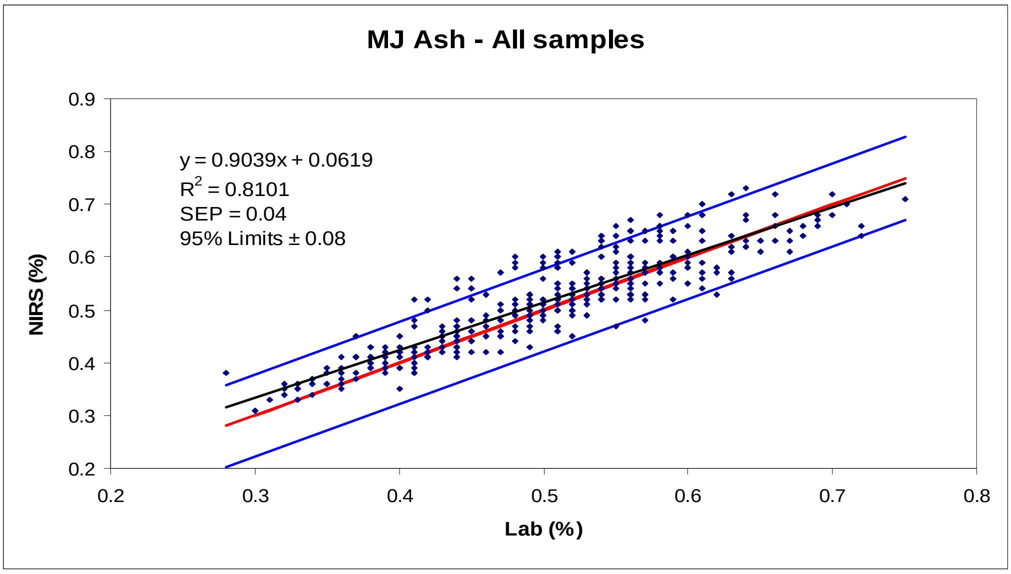


Figure 3. Scatter plot of near infra-red spectroscopy (NIRS) predictions for mixed juice conductivity ash.

Again due to the low ash concentration (0.3 to 0.7%) and the generally small range in the ash values from each factory, NIRS precision made RSQ values for all individual factories poor (see Appendix 6). Differences between the laboratory and NIRS values of 0.09 to 0.11% were regularly observed. It was noted that NIRS predictions improved throughout the season as the calibration was expanded. Data from week 27 onwards gave good correlation statistics (slope 0.98 and RSQ 0.98) with no bias.

Molasses

Molasses quality control

Forty batches of the three molasses control samples were tested during the period of study. No results fell within warning or action areas for any property. The use of controls also proved useful when the MPA source lamp was replaced during the season. No differences in performance were observed, without the need for calibration adjustment.

Molasses overall results

The results presented in Table 2 show the correlation between laboratory and NIRS results from weeks 23 to 43 of the 2007-2008 season. Individual results were excluded as outliers where they exceeded three times the standard deviation from the mean lab-NIRS value.

Table 2. Summary of near infra-red spectrometer (NIRS) performance for molasses (all samples).

Analyte (unit)	Sample count	Outliers removed	SEP (%)	Slope	Bias	RSQ	95% confidence limits (%)	Lab method tolerance (%)
Brix (°Bx)	430	7	0.37	0.98	-0.22	0.98	± 0.72	± 0.45
Pol (°Z)	433	3	0.45	0.96	-0.04	0.96	± 0.88	± 0.20
Sucrose (%)	436	1	0.7	0.89	-0.1	0.89	± 1.3	± 0.6
Fructose (%)	427	2	0.3	0.98	-0.1	0.93	± 0.5	± 0.3
Glucose (%)	430	2	0.3	0.95	0.0	0.96	± 0.6	± 0.3
Conductivity ash (%)	435	2	0.24	1.01	-0.02	0.99	± 0.48	± 0.15
Dry solids (%)	435	2	0.40	0.95	0.0	0.97	± 0.78	± 0.50
TPD	438	3	1.0	0.96	-0.2	0.92	± 1.9	± 1.3*
Hybrid TPD	439	2	0.3	0.98	0.0	0.96	± 0.5	± 1.3*

SEP = standard error of prediction, RSQ = correlation coefficient squared, * = calculated

The NIRS predictive capability for each mixed juice property is summarised for each factory in Appendix 7-15.

Molasses Brix

The Brix data from Table 2 are represented graphically in Figure 4, which shows the regression lines, slope and 95% confidence limits. This showed very good slope, SEP and RSQ statistics of 0.98, 0.37 and 0.98, respectively. A bias value of -0.22 showed a general over-estimation by the NIRS. This was also evidenced by most of the individual factories also showing a negative bias (Appendix 7). Nonetheless, the 95% confidence intervals show most NIRS results to be within 0.72% of the laboratory generated result. This was true even for very high Brix UK samples (>85% Bx) where the dry solids were determined by the vacuum oven dry solids method. Removing these results improved the slope and removed the bias otherwise associated with UK. The three individual factories with by far the worst SEP values (0.6 to 1.2%) were all outside South Africa (MH, SM and MW).

Molasses pol

Pol, as with sucrose (discussed below), is affected by the varying ratios of sucrose and monosaccharides, and the NIRS predictions are thus less precise than for Brix. The SEP value of 0.45 is more than twice the laboratory tolerance of 0.20%, giving a relatively wide 95% confidence interval of 0.88%. The slope, RSQ and bias figures of 0.96, 0.96 and -0.04, respectively, are nonetheless acceptable (Figure 5).

Some individual factories showed consistent over- or under-predictions of up to 0.4% for South African factories, and up to 0.5% for non-South African factories (Appendix 8).

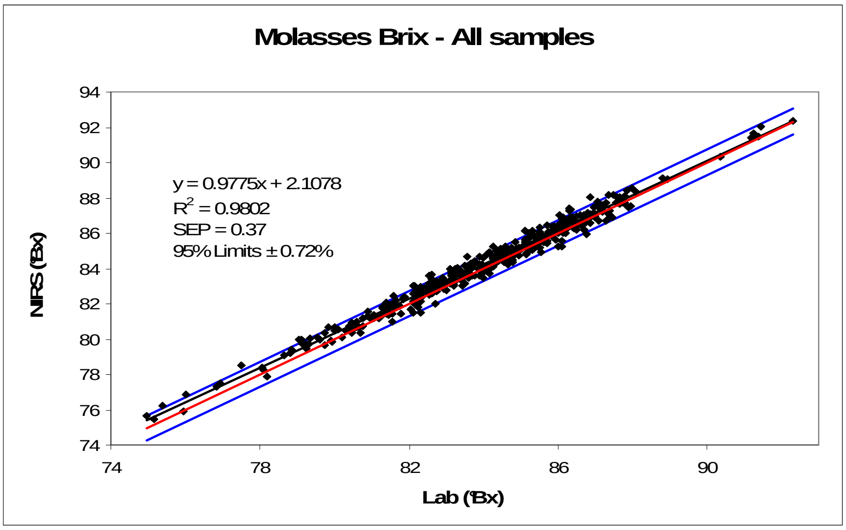


Figure 4. Scatter plot of near infra-red spectroscopy (NIRS) predictions for molasses Brix.

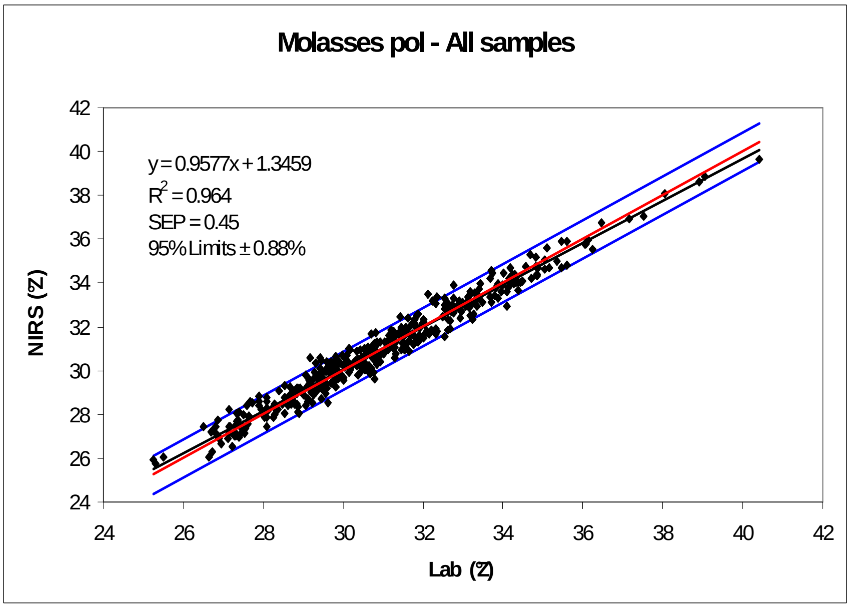


Figure 5. Scatter plot of near infra-red spectroscopy (NIRS) predictions for molasses pol.

Molasses sucrose

NIRS estimation of pol and sucrose in low purity samples is adversely affected by the contribution of the monosaccharides. The calibration set is unlikely to account for all possible combinations of fructose, glucose and sucrose. The three analytes also share overlapping spectral bands. In addition, sucrose reference data in the calibration is also obtained by the HPAEC method with a wide tolerance of 0.6%. Sucrose predictions were thus relatively poor (SEP=0.7%, slope=0.89, RSQ=0.89) (Figure 6).

In addition some individual factories showed consistent bias, with NIRS over-predicting the sucrose by between 0.2 and 0.5% (Appendix 9). A bias-free but poor RSQ of 0.4 for MS is evidence of the scatter caused by the relatively poor NIRS precision. AK, UC and ES all showed over-predictions of 0.4 to 0.5% sucrose. It is evident from the SEP values that the South African factories are generally better predicted than the non-South African factories.

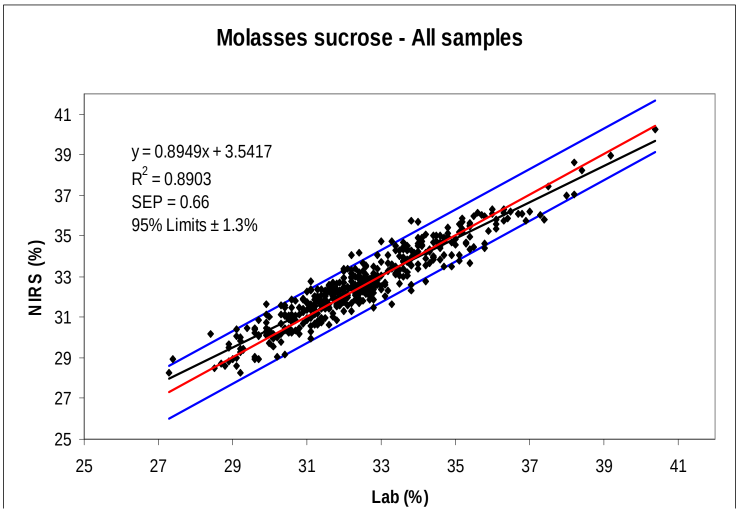
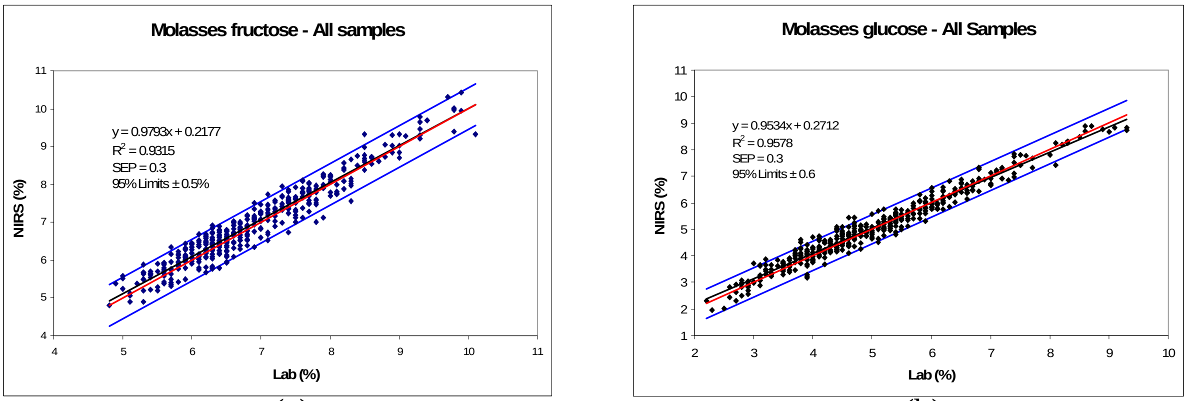


Figure 6. Scatter plot of near infra-red spectroscopy (NIRS) predictions for molasses sucrose.

Molasses fructose and glucose

Both fructose and glucose were predicted well by NIRS, with slopes of 0.95 and 0.98, and RQS values of 0.96 and 0.93, respectively. The SEP values were better than the laboratory method tolerances, with only fructose showing any sign of bias with an average over-estimation of 0.1%. Figure 7(a,b) shows overall data for fructose and glucose from Table 2.



(a) (b)

Figure 7(a,b). Scatter plot of near infra-red spectroscopy (NIRS) predictions for molasses fructose and glucose.

No individual factories showed bias of more than 0.2% for fructose (Appendix 11). For glucose (Appendix 10), NB and MH offset each other in the total analysis with a bias of -0.4 and +0.4%, respectively. Only ES showed a relatively poor RSQ of 0.35 for fructose. This may be partly attributable to the narrow range (1.1% fructose) recorded in the period of study, although no differences between the laboratory and NIRS values were greater than 0.5%.

Molasses conductivity ash

Slope, RSQ and bias values of 1.01, 0.99 and -0.02%, respectively, show excellent sensitivity and linearity, with the SEP of 0.24 comparing well with the laboratory method tolerance of 0.15% (Figure 8).

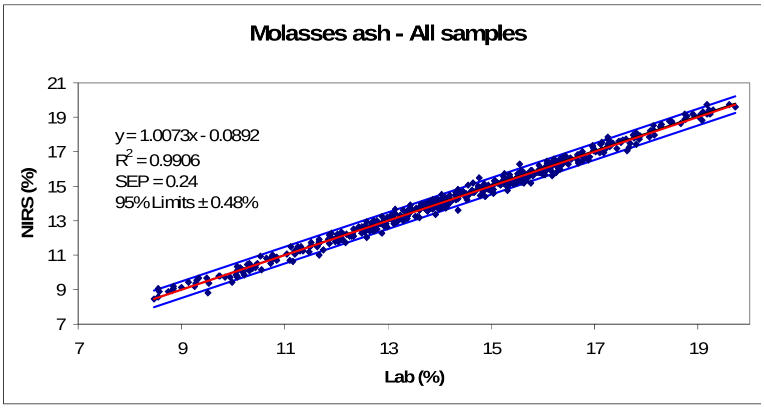


Figure 8. Scatter plot of near infra-red spectroscopy (NIRS) predictions for molasses conductivity ash.

Individual mill performance was good (Appendix 12). MA showed a general under-estimation of 0.5%, with no other factories having positive or negative bias of more than 0.3%. As noted with Brix and sucrose above, the South African factories were better predicted than non-South African factories, with SEP values for MA, UB and MH more than twice the values of those for South African factories.

Molasses dry solids

The NIRS predictive capability for dry solids is very similar in performance to Brix, but with no bias present (slope=0.95, RSQ=0.97, bias=0.00). SEP at 0.40 is better than the laboratory tolerance of 0.50% (Figure 9). Individual factory performances were good (Appendix 13).

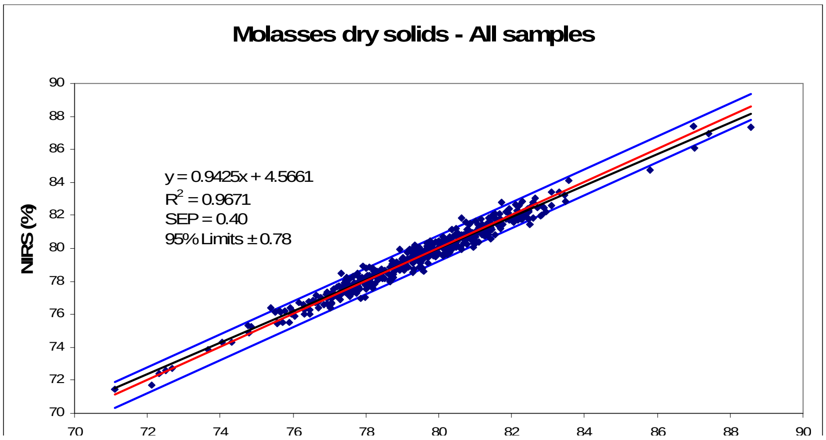


Figure 9. Scatter plot of near infra-red spectroscopy (NIRS) predictions for molasses dry solids.

Molasses TPD

The maximum error in the calculated TPD is 1.3 units (calculated from the maximum error associated with each of the contributing laboratory results) (Figure 10). TPD when calculated from individual NIRS predicted values was poor. A large SEP of 1.0 and 95% confidence interval of 1.9 made this unacceptable, with the effect of relatively poor sucrose predictions identified as a primary cause.

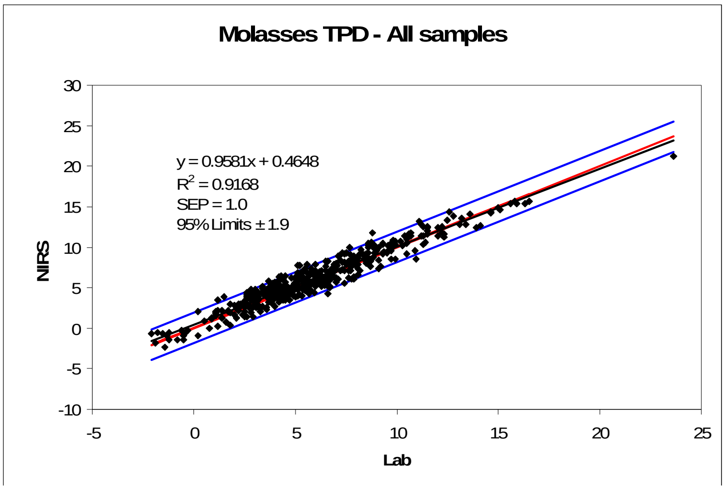


Figure 10. Scatter plot of near infra-red spectroscopy (NIRS) predictions for molasses target purity difference (TPD) (calculated from all NIRS results).

Hybrid TPD

Hybrid TPD used only the dry solids and ash as predicted by NIRS, and retained the laboratory-generated results for fructose, glucose and sucrose. The excellent predictions for ash and dry solids resulted in very good Hybrid TPD correlations with the laboratory-calculated TPD (slope=0.98, RSQ=0.96, bias=0.0) (Figure 11). The SEP and confidence intervals were also excellent, with 95% of Hybrid TPD results differing from the laboratory figure by less than 0.5 units. In addition, none of the factories showed any positive or negative bias of more than 0.2 units (Appendix 15).

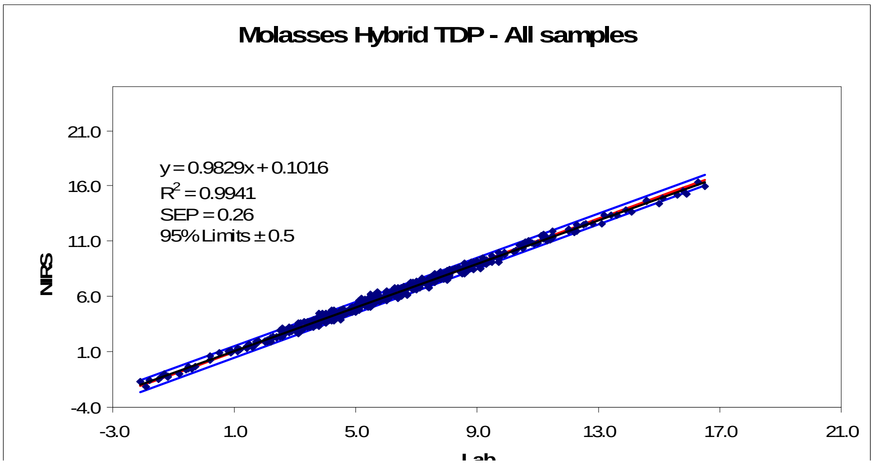


Figure 11. Scatter plot of near infra-red spectroscopy (NIRS) predictions for molasses Hybrid target purity difference (TPD).

Recommendations

It is recommended that the improvement of the NIRS predictions for molasses samples, with special focus on sucrose and TPD, be further investigated. Increasing the number of replicate measurements from two to three may improve the averaging precision, but the actual precision of each measurement also needs improvement. More stringent temperature control could be achieved by using a temperature control attachment to the NIRS. Currently all samples are scanned at a laboratory-controlled temperature of 20°C, but this could be slightly elevated to allow control at factory laboratory conditions. Current calibrations could be split into two or more calibration sets more specific to geographical regions or other identifiable commonalities. All calibrations should be continually monitored and where necessary updated to include spectra that may help to further improve their robustness to different sample compositions. Inter-instrument transferability of the calibrations still needs investigation.

Conclusions

Mixed juice
The NIRS predictions for Brix, pol and sucrose compare excellently with the laboratory-generated results. Fructose and glucose are predicted linearly across their overall concentration ranges. The proportionally large tolerance in the laboratory result precision causes scatter in the NIRS results; however, all NIRS results still fall within 0.06% of the laboratory values. Although conductivity ash was relatively poorly predicted, the predictions improved throughout the season as more spectra were included in the calibration. The last 16 weeks produced acceptable bias-free results.

Molasses
NIRS predictions for molasses conductivity ash and dry solids are excellent across all factories. In general, Brix is slightly over-predicted by 0.2% Brix, but showed good linearity even above 85°Bx. Predictions for pol are linear and without bias, but the prediction error is more than twice the laboratory precision. Fructose and glucose are predicted well, with prediction errors better than the laboratory method precision. Some individual factories showed bias of up to ±0.4% for glucose.

Molasses sucrose predictions were relatively poor and further work is needed for this analyte. Calculating molasses TPD using individual NIRS predicted results is poor and not feasible at this time. Hybrid TPD can be calculated using the NIRS predicted ash and dry solids results, and laboratory method results for fructose, glucose and sucrose. This Hybrid TPD correlates very well with the laboratory-calculated TPD values. NIRS generally predicts molasses results more accurately for South African versus non-South African factories.

General
The calibrations do not need updating when the MPA source lamp is replaced.

Acknowledgements

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Appendix 1. Mixed juice Brix performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	21	1.00	1.00	-0.01	3.91	0.04
Komati 1	21	0.99	1.00	0.04	4.66	0.03
Komati 2	20	0.99	1.00	0.02	3.60	0.02
Pongola	21	0.98	1.00	0.01	3.30	0.04
Umfolozi	20	0.97	1.00	0.01	3.19	0.04
Felixton 1	20	1.00	0.99	-0.05	2.27	0.05
Felixton 2	18	1.01	1.00	0.02	3.97	0.05
Amatikulu	19	0.98	1.00	0.01	1.99	0.03
Darnall	20	0.98	1.00	-0.02	2.64	0.05
Maidstone 1	17	0.99	1.00	0.02	4.47	0.05
Maidstone 2	18	0.98	1.00	0.00	4.22	0.04
Gledhow 1	20	0.98	1.00	0.01	4.19	0.05
Gledhow 2	20	0.99	1.00	-0.06	3.59	0.04
Noodsberg	21	0.98	0.99	-0.05	3.39	0.08
UCL Co. Ltd	20	1.00	1.00	0.01	2.53	0.04
Eston	21	0.99	1.00	0.00	3.99	0.05
Sezela 1	21	0.99	1.00	-0.02	4.28	0.05
Sezela 2	21	0.99	1.00	-0.01	4.82	0.05
Umzimkulu	21	0.99	1.00	-0.01	3.71	0.04
Nchalo	14	1.00	1.00	-0.07	3.07	0.06
Nakambala 1	19	0.99	1.00	0.02	2.87	0.05
Nakambala 2	19	0.96	1.00	-0.05	1.67	0.04

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 2. Mixed juice pol performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	21	1.01	1.00	0.02	3.70	0.03
Komati 1	21	0.98	1.00	0.02	4.32	0.05
Komati 2	20	1.02	1.00	-0.03	3.24	0.03
Pongola	21	1.01	1.00	0.01	3.25	0.04
Umfolozi	20	0.97	1.00	0.02	3.24	0.05
Felixton 1	19	0.98	1.00	-0.01	2.51	0.05
Felixton 2	18	1.00	1.00	-0.01	4.13	0.07
Amatikulu	19	0.98	1.00	0.02	2.07	0.03
Darnall	20	0.96	0.99	0.01	2.84	0.08
Maidstone 1	17	0.95	1.00	0.06	4.19	0.08
Maidstone 2	18	0.96	1.00	0.00	4.01	0.06
Gledhow 1	20	0.97	1.00	0.03	4.45	0.06
Gledhow 2	20	0.99	1.00	-0.04	3.86	0.05
Noodsberg	21	1.02	0.99	-0.09	3.43	0.08
UCL Co. Ltd	20	1.00	1.00	0.02	2.37	0.04
Eston	21	0.97	1.00	0.06	3.87	0.04
Sezela 1	21	0.97	1.00	0.04	4.04	0.07
Sezela 2	21	0.96	1.00	0.03	4.54	0.07
Umzimkulu	21	0.96	1.00	0.00	3.89	0.07
Nchalo	14	1.03	1.00	-0.08	3.36	0.07
Nakambala 1	19	1.02	0.99	0.06	2.83	0.07
Nakambala 2	19	1.05	0.98	0.02	1.38	0.06

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 3. Mixed juice sucrose performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	20	1.02	1.00	0.03	3.72	0.05
Komati 1	20	1.02	1.00	0.02	4.14	0.05
Komati 2	19	1.02	1.00	-0.01	3.28	0.05
Pongola	20	1.02	1.00	-0.02	3.17	0.04
Umfolozi	19	0.98	1.00	0.01	3.18	0.04
Felixton 1	18	1.01	0.99	-0.03	2.32	0.06
Felixton 2	17	0.98	1.00	0.00	4.08	0.06
Amatikulu	18	0.97	1.00	0.01	2.05	0.05
Darnall	19	0.95	1.00	0.00	2.71	0.07
Maidstone 1	16	0.96	1.00	0.03	4.15	0.06
Maidstone 2	17	0.97	1.00	-0.03	3.95	0.06
Gledhow 1	19	0.98	1.00	0.02	4.33	0.05
Gledhow 2	19	0.97	1.00	-0.03	3.83	0.06
Noodsberg	20	1.01	0.99	-0.08	3.40	0.08
UCL Co. Ltd	19	0.99	1.00	0.03	2.32	0.05
Eston	20	0.98	1.00	0.03	3.80	0.05
Sezela 1	20	0.98	1.00	0.00	3.92	0.04
Sezela 2	20	0.98	1.00	0.00	4.41	0.05
Umzimkulu	20	0.98	1.00	-0.02	3.74	0.05
Nchalo	13	1.01	1.00	-0.01	3.32	0.05
Nakambala 1	18	1.02	0.99	0.04	2.87	0.08
Nakambala 2	18	1.05	0.97	-0.01	1.34	0.07

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 4. Mixed juice fructose performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	21	1.17	0.74	-0.01	0.13	0.02
Komati 1	21	1.07	0.79	-0.01	0.15	0.02
Komati 2	20	1.16	0.78	-0.01	0.14	0.03
Pongola	21	1.24	0.71	0.00	0.11	0.03
Umfolozi	20	1.05	0.87	-0.01	0.15	0.02
Felixton 1	20	0.93	0.92	0.00	0.31	0.02
Felixton 2	18	0.64	0.58	0.00	0.13	0.03
Amatikulu	19	1.08	0.90	-0.01	0.13	0.02
Darnall	20	0.89	0.70	0.00	0.15	0.02
Maidstone 1	17	0.67	0.14	-0.01	0.05	0.02
Maidstone 2	18	1.04	0.46	0.00	0.06	0.02
Gledhow 1	20	0.94	0.80	-0.01	0.15	0.02
Gledhow 2	20	0.76	0.80	-0.01	0.17	0.02
Noodsberg	21	0.88	0.75	0.01	0.12	0.02
UCL Co. Ltd	20	1.25	0.79	0.00	0.08	0.02
Eston	21	0.87	0.45	0.00	0.08	0.02
Sezela 1	21	0.61	0.57	0.00	0.10	0.02
Sezela 2	21	0.91	0.68	0.01	0.09	0.02
Umzimkulu	20	0.90	0.54	0.02	0.10	0.02
Nchalo	14	1.15	0.88	0.01	0.10	0.02
Nakambala 1	19	0.88	0.68	0.01	0.20	0.03
Nakambala 2	18	0.89	0.79	0.02	0.23	0.03

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 5. Mixed juice glucose performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	20	0.83	0.83	0.01	0.17	0.02
Komati 1	20	0.92	0.86	0.00	0.16	0.02
Komati 2	19	0.89	0.86	0.01	0.17	0.02
Pongola	20	1.10	0.80	0.00	0.12	0.02
Umfolozi	19	1.08	0.81	0.01	0.15	0.02
Felixton 1	19	1.07	0.92	0.00	0.22	0.02
Felixton 2	17	0.77	0.81	0.02	0.16	0.02
Amatikulu	18	0.93	0.84	0.00	0.13	0.02
Darnall	19	0.95	0.83	0.00	0.19	0.02
Maidstone 1	16	0.65	0.18	-0.01	0.04	0.02
Maidstone 2	17	0.26	0.11	0.00	0.09	0.02
Gledhow 1	19	0.88	0.72	0.00	0.15	0.02
Gledhow 2	19	0.78	0.79	0.01	0.16	0.02
Noodsberg	20	0.63	0.30	-0.01	0.10	0.03
UCL Co. Ltd	19	0.10	0.00	-0.01	0.07	0.03
Eston	20	0.87	0.57	-0.01	0.07	0.02
Sezela 1	20	0.70	0.41	0.01	0.06	0.02
Sezela 2	20	0.63	0.50	0.00	0.11	0.02
Umzimkulu	20	0.92	0.59	0.02	0.09	0.02
Nchalo	13	0.96	0.89	0.00	0.14	0.02
Nakambala 1	18	0.94	0.67	0.01	0.21	0.03
Nakambala 2	17	0.84	0.75	0.01	0.22	0.03

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 6. Mixed juice conductivity ash performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	20	1.24	0.42	-0.03	0.10	0.04
Komati 1	18	0.56	0.19	0.00	0.11	0.04
Komati 2	19	0.42	0.13	0.00	0.14	0.05
Pongola	20	0.78	0.36	0.00	0.15	0.05
Umfolozi	19	1.10	0.55	-0.01	0.12	0.04
Felixton 1	19	0.89	0.36	-0.03	0.12	0.04
Felixton 2	17	1.29	0.59	0.00	0.12	0.04
Amatikulu	18	1.02	0.50	-0.01	0.11	0.03
Darnall	19	1.24	0.48	-0.02	0.12	0.04
Maidstone 1	16	1.11	0.62	-0.01	0.15	0.04
Maidstone 2	17	1.15	0.64	-0.02	0.13	0.04
Gledhow 1	19	0.95	0.70	-0.02	0.19	0.04
Gledhow 2	19	1.18	0.57	-0.02	0.11	0.04
Noodsberg	19	1.05	0.57	-0.01	0.12	0.04
UCL Co. Ltd	19	0.94	0.54	-0.02	0.12	0.04
Eston	19	1.10	0.64	-0.03	0.12	0.04
Sezela 1	20	1.22	0.74	-0.03	0.14	0.04
Sezela 2	20	1.03	0.70	-0.02	0.19	0.04
Umzimkulu	19	1.07	0.39	-0.03	0.09	0.04
Nchalo	13	0.53	0.61	0.01	0.30	0.05
Nakambala 1	17	0.88	0.27	0.00	0.15	0.05
Nakambala 2	18	1.24	0.56	-0.01	0.13	0.04

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 7. Molasses Brix performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	20	0.97	0.95	-0.42	4.10	0.27
Komati	19	0.92	0.80	-0.32	2.75	0.41
Pongola	21	1.09	0.96	-0.37	4.30	0.29
Umfolozi	19	0.98	0.99	-0.41	11.25	0.32
Amatikulu	19	1.07	0.93	-0.16	3.95	0.37
Felixton	18	0.93	0.93	-0.03	2.85	0.23
Gledhow	19	0.97	0.98	-0.36	7.90	0.30
Darnall	17	0.97	0.93	-0.13	5.80	0.39
Maidstone	17	1.08	0.98	0.11	7.35	0.34
UCL Co. Ltd	20	1.00	0.96	-0.33	5.45	0.34
Noodsberg	19	1.04	0.96	-0.43	6.50	0.37
Eston	21	0.91	0.87	-0.01	4.35	0.38
Sezela	19	0.93	0.97	-0.22	6.75	0.33
Umzimkulu	20	0.94	0.99	-0.38	9.75	0.33
Dwangwa	18	0.98	0.90	-0.35	3.75	0.36
Ruembe	19	1.02	0.92	-0.14	3.25	0.28
Nchalo	15	0.94	0.98	-0.20	6.85	0.38
Nakambala	17	0.87	0.93	-0.11	5.90	0.38
Maragra	20	0.91	0.96	-0.17	6.15	0.35
Ubombo	20	0.91	0.91	-0.09	3.70	0.35
Mhlume	16	0.98	0.94	0.35	5.55	1.19
Simunye	17	1.01	0.96	0.09	6.50	0.73
Msolwa	20	0.93	0.97	0.05	9.05	0.59

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 8. Molasses pol performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	21	1.00	0.98	-0.11	10.70	0.33
Komati	19	1.11	0.94	0.02	4.08	0.46
Pongola	21	0.97	0.99	0.00	9.36	0.38
Umfolozi	19	1.10	0.91	-0.42	6.40	0.57
Amatikulu	19	1.02	0.96	-0.33	4.40	0.25
Felixton	18	0.98	0.94	-0.19	3.98	0.27
Gledhow	20	0.85	0.90	0.38	4.55	0.38
Darnall	18	0.83	0.84	0.08	2.55	0.34
Maidstone	17	1.03	0.92	0.01	3.24	0.25
UCL Co. Ltd	21	0.97	0.98	-0.05	6.80	0.39
Noodsberg	20	0.97	0.98	-0.08	9.06	0.45
Eston	21	0.96	0.97	-0.14	5.24	0.29
Sezela	20	0.88	0.93	0.12	6.39	0.51
Umzimkulu	21	0.88	0.87	0.09	3.79	0.37
Dwangwa	18	0.95	0.93	-0.30	4.63	0.32
Ruembe	19	0.97	0.96	0.00	7.22	0.42
Nchalo	15	0.93	0.97	-0.26	4.72	0.26
Nakambala	16	1.20	0.92	0.14	3.79	0.41
Maragra	17	1.05	0.94	-0.19	6.80	0.50
Ubombo	20	0.96	0.96	0.56	9.75	0.43
Mhlume	16	0.96	0.93	0.26	5.70	0.38
Simunye	17	0.97	0.88	-0.53	4.33	0.36
Msolwa	20	0.86	0.86	-0.36	5.37	0.54

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 9. Molasses sucrose performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	21	0.90	0.91	0.3	8.0	0.6
Komati	19	0.87	0.70	0.1	3.1	0.5
Pongola	21	0.87	0.95	-0.2	8.2	0.6
Umfolozi	19	0.84	0.81	-0.2	5.5	0.6
Amatikulu	19	0.84	0.84	-0.4	3.7	0.5
Felixton	18	0.73	0.82	0.0	4.2	0.5
Gledhow	20	1.02	0.72	-0.1	3.1	0.5
Darnall	18	0.82	0.58	0.1	2.4	0.5
Maidstone	17	0.70	0.41	0.0	2.9	0.7
UCL Co. Ltd	21	0.75	0.81	-0.4	6.5	0.8
Noodsberg	20	0.85	0.87	-0.3	6.8	0.7
Eston	21	0.71	0.71	-0.5	3.6	0.7
Sezela	20	1.00	0.86	0.0	5.9	0.6
Umzimkulu	21	0.79	0.80	-0.1	5.2	0.6
Dwangwa	18	0.51	0.72	0.1	4.4	0.8
Ruembe	19	0.81	0.81	0.1	6.2	0.8
Nchalo	15	0.76	0.78	0.1	5.1	0.7
Nakambala	17	0.71	0.57	0.1	3.7	0.8
Maragra	20	0.91	0.78	0.0	5.8	0.8
Ubombo	20	0.88	0.84	0.3	7.2	0.6
Mhlume	16	0.60	0.67	-0.2	4.9	0.7
Simunye	17	0.66	0.69	0.0	4.6	0.7
Msolwa	19	0.74	0.88	-0.3	5.6	0.6

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 10. Molasses glucose performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	21	0.95	0.88	0.1	2.4	0.3
Komati	19	0.93	0.93	0.2	2.5	0.2
Pongola	21	0.95	0.94	0.0	2.8	0.2
Umfolozi	19	0.94	0.98	0.0	3.4	0.2
Amatikulu	19	0.96	0.92	-0.1	2.8	0.2
Felixton	18	1.22	0.87	0.2	1.7	0.3
Gledhow	20	1.09	0.94	0.0	2.0	0.2
Darnall	18	1.01	0.90	-0.1	2.3	0.2
Maidstone	17	1.15	0.85	-0.1	1.3	0.2
UCL Co. Ltd	18	1.50	0.92	-0.1	1.9	0.4
Noodsberg	20	1.03	0.81	-0.4	2.0	0.2
Eston	20	1.21	0.86	-0.1	1.7	0.2
Sezela	20	0.99	0.95	-0.1	1.7	0.1
Umzimkulu	20	0.81	0.90	-0.2	2.0	0.2
Dwangwa	18	0.88	0.86	-0.1	1.6	0.2
Ruembe	18	0.93	0.97	-0.1	4.6	0.2
Nchalo	15	0.87	0.92	-0.2	2.4	0.2
Nakambala	17	0.94	0.96	-0.2	3.8	0.3
Maragra	20	0.94	0.88	-0.1	2.6	0.3
Ubombo	20	0.92	0.89	0.1	1.8	0.2
Mhlume	16	1.09	0.95	0.4	2.7	0.2
Simunye	17	0.98	0.84	0.0	1.6	0.2
Msolwa	19	0.72	0.88	-0.2	3.3	0.4

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 11. Molasses fructose performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	20	1.01	0.92	-0.1	2.2	0.2
Komati	19	1.07	0.94	-0.1	2.3	0.2
Pongola	20	0.82	0.85	0.2	2.4	0.3
Umfolozi	18	0.99	0.97	0.0	2.9	0.2
Amatikulu	19	0.82	0.77	0.0	2.6	0.3
Felixton	18	0.83	0.70	-0.1	1.7	0.3
Gledhow	20	0.87	0.76	0.0	1.5	0.2
Darnall	18	0.61	0.73	-0.1	1.5	0.3
Maidstone	17	0.68	0.61	-0.1	1.7	0.3
UCL Co. Ltd	20	0.81	0.78	-0.1	1.8	0.2
Noodsberg	20	0.75	0.86	-0.1	2.6	0.2
Eston	20	0.76	0.35	0.0	1.1	0.3
Sezela	20	0.57	0.85	-0.1	2.1	0.4
Umzimkulu	20	0.74	0.92	0.1	2.3	0.3
Dwangwa	17	1.28	0.77	0.1	1.7	0.3
Ruembe	18	1.09	0.91	0.0	3.5	0.4
Nchalo	15	1.28	0.94	0.1	1.7	0.2
Nakambala	17	1.22	0.94	0.0	2.5	0.3
Maragra	20	1.16	0.84	0.0	2.0	0.3
Ubombo	20	0.92	0.90	-0.1	2.7	0.2
Mhlume	16	1.03	0.95	-0.2	2.3	0.2
Simunye	17	0.92	0.81	0.1	2.1	0.3
Msolwa	18	0.87	0.63	-0.1	1.9	0.4

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 12. Molasses conductivity ash performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	21	1.07	0.97	-0.15	4.14	0.22
Komati	19	1.11	0.95	-0.06	2.53	0.23
Pongola	21	1.00	0.98	-0.02	5.73	0.21
Umfolozi	19	1.06	1.00	0.03	7.75	0.24
Amatikulu	19	0.96	0.97	-0.09	3.42	0.18
Felixton	18	1.08	0.97	-0.11	3.62	0.22
Gledhow	20	1.06	0.98	0.05	4.26	0.24
Darnall	18	1.07	0.98	-0.13	4.36	0.23
Maidstone	17	1.06	0.96	-0.08	3.28	0.21
UCL Co. Ltd	20	1.03	0.99	0.20	4.84	0.21
Noodsberg	20	0.97	0.98	0.26	4.96	0.22
Eston	21	1.00	0.97	-0.12	3.46	0.19
Sezela	20	0.92	0.91	0.06	2.67	0.24
Umzimkulu	21	0.93	0.92	0.10	3.33	0.27
Dwangwa	17	0.85	0.86	0.13	1.95	0.20
Ruembe	19	0.93	0.98	-0.03	4.56	0.19
Nchalo	15	1.04	0.94	0.04	3.06	0.23
Nakambala	17	1.05	0.99	-0.04	6.91	0.24
Maragra	20	1.02	0.99	0.51	4.50	0.75
Ubombo	20	0.97	0.94	0.07	3.65	0.46
Mhlume	16	1.08	0.96	0.24	2.88	0.63
Simunye	17	1.06	0.94	-0.27	2.15	0.16
Msolwa	20	0.96	0.98	0.03	3.55	0.31

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 13. Molasses dry solids performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	21	0.82	0.90	0.05	3.35	0.32
Komati	19	0.87	0.84	0.06	2.75	0.30
Pongola	21	0.79	0.80	0.18	3.75	0.47
Umfolozi	19	0.96	0.99	0.01	9.87	0.35
Amatikulu	19	0.94	0.78	0.01	3.11	0.43
Felixton	18	0.93	0.82	-0.09	1.98	0.29
Gledhow	20	0.90	0.94	0.03	7.33	0.38
Darnall	18	0.84	0.90	0.10	4.01	0.32
Maidstone	17	0.90	0.95	0.28	7.17	0.39
UCL Co. Ltd	21	0.92	0.87	0.11	3.92	0.39
Noodsberg	20	0.88	0.85	-0.06	4.63	0.43
Eston	21	0.89	0.69	0.01	3.00	0.44
Sezela	20	0.91	0.94	0.02	5.44	0.32
Umzimkulu	19	0.90	0.98	0.19	9.15	0.51
Umzimkulu*	15	0.94	0.85	-0.01	2.23	0.30
Dwangwa	18	1.00	0.90	0.07	3.49	0.32
Ruembe	19	0.99	0.94	-0.16	3.59	0.28
Nchalo	15	0.91	0.94	0.31	5.66	0.49
Nakambala	17	0.74	0.75	0.18	3.70	0.52
Maragra	20	0.92	0.94	-0.07	4.89	0.35
Ubombo	20	0.74	0.74	0.26	3.44	0.48
Mhlume	16	0.95	0.88	-0.17	5.10	0.47
Simunye	17	0.91	0.93	-0.17	6.13	0.42
Msolwa	20	1.01	0.97	-0.01	8.37	0.33

RSQ = correlation coefficient squared, SEP = standard error of prediction
*=UK with four samples above 85% Brix tested by vacuum oven dry solids removed

Appendix 14. Molasses TPD performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	21	0.89	0.91	0.4	11.6	0.9
Komati	19	0.60	0.35	0.1	2.8	0.7
Pongola	22	0.87	0.97	-0.3	20.8	0.8
Umfolozi	19	1.11	0.96	-0.3	12.5	0.9
Amatikulu	18	0.83	0.58	-0.6	3.9	0.7
Felixton	18	0.74	0.72	0.1	5.2	0.8
Gledhow	20	0.69	0.54	-0.3	3.8	0.8
Darnall	18	0.66	0.63	0.0	4.8	0.7
Maidstone	17	0.60	0.36	-0.2	4.7	0.9
UCL Co. Ltd	21	0.92	0.89	-0.7	11.2	1.2
Noodsberg	20	0.94	0.93	-0.8	12.4	0.9
Eston	20	0.86	0.83	-0.5	5.9	0.9
Sezela	20	0.83	0.64	-0.1	5.8	0.9
Umzimkulu	21	0.63	0.52	-0.4	4.8	0.8
Dwangwa	18	0.25	0.17	0.1	4.1	1.3
Ruembe	19	0.86	0.87	0.2	10.6	1.0
Nchalo	15	0.56	0.31	-0.1	3.6	1.0
Nakambala	17	1.15	0.75	-0.1	6.6	1.1
Maragra	20	1.01	0.81	-0.1	7.3	1.1
Ubombo	20	0.84	0.85	0.4	9.9	0.9
Mhlume	16	0.67	0.56	-0.1	5.9	1.1
Simunye	18	0.25	0.18	0.3	3.9	1.1
Msolwa	20	0.60	0.51	-0.5	4.4	0.8

RSQ = correlation coefficient squared, SEP = standard error of prediction

Appendix 15. Molasses Hybrid TPD performance per factory.

Factory	Count	Slope	RSQ	Bias	Range (%)	SEP (%)
Malalane	21	0.97	1.00	0.0	11.6	0.2
Komati	19	1.09	0.95	0.0	2.8	0.2
Pongola	21	0.96	0.99	-0.1	13.1	0.3
Umfolozi	19	1.01	1.00	0.0	12.5	0.2
Amatikulu	19	0.99	0.94	0.0	3.9	0.2
Felixton	18	0.98	0.99	0.1	5.2	0.2
Gledhow	20	0.96	0.96	0.0	3.8	0.2
Darnall	18	1.00	0.98	0.0	4.8	0.2
Maidstone	17	0.88	0.98	-0.1	4.7	0.2
UCL Co. Ltd	21	0.99	1.00	-0.2	11.2	0.2
Noodsberg	20	0.97	0.99	-0.1	12.4	0.3
Eston	21	0.98	0.98	0.0	5.9	0.3
Sezela	20	0.97	0.97	0.0	5.8	0.2
Umzimkulu	20	0.92	0.89	-0.2	4.1	0.4
Dwangwa	18	0.99	0.98	-0.1	4.1	0.2
Ruembe	21	0.98	0.99	0.1	10.6	0.2
Nchalo	15	0.93	0.91	-0.2	3.6	0.3
Nakambala	17	0.95	0.96	-0.1	6.6	0.3
Maragra	20	0.96	0.99	-0.1	7.3	0.2
Ubombo	20	0.92	0.98	-0.1	9.9	0.3
Mhlume	16	0.94	0.97	0.1	5.9	0.3
Simunye	18	0.93	0.97	0.2	3.9	0.2
Msolwa	21	1.00	0.96	0.1	4.4	0.3

RSQ = correlation coefficient squared, SEP = standard error of prediction