RECONCILIATION OF PROCESS FLOW RATES FOR A STEADY STATE MASS BALANCE ON A CENTRIFUGAL

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Abstract

When evaluating the performance of a centrifugal, the flows and compositions of the streams entering and leaving the unit must be known. It is not necessary (nor easy) to measure all flows and compositions but the unknown quantities can be calculated by steady state mass balance from a minimum number of measurements. If more than the minimum number of measurements are available, a means must be found to reconcile the inevitable discrepancies between different ways of calculating unmeasured quantities. Published mathematical techniques have described how to achieve the 'best fit' to the available data and provide an adjusted data set which reconciles the probable measurement errors with the requirements of mass balance. These methods were adapted to allow them to be applied using a simple spreadsheet calculation.

Introduction

Sometimes the apparently mundane prompts a question of unexpected depth. Answering the question can provide equally deep insights with wider application. This was the situation encountered in testing a new design of continuous A-centrifugal at Darnall. The capacity of the centrifugal needed to be quantified in terms of the quantity of massecuite that it was able to process. Massecuite flow is particularly difficult to measure directly on a factory scale but is easily estimated from other flow measurements and laboratory analyses (which are in any case required to analyse the centrifugal's performance) by applying a simple mass balance.

The attraction of this approach is rapidly dispelled when a few sample calculations demonstrate that significantly different answers for the estimated massecuite flow rate are obtained, depending on the type of mass balance used and the consequent sub-set of the available measurements which are used in the calculation. This is a situation where a surplus of information highlights uncertainty rather than providing a confirmation of results. A survey of the literature shows that this type of problem (known as the reconciliation of process flows) has been the subject of significant academic study. The challenge was thus to find an appropriate way of applying the solutions of the generalised problems presented in the literature to the specific requirements of evaluating a continuous A-centrifugal. A good practical solution to this problem could have much wider application in the sugar industry and would justify this deeper investigation into an apparently simple flow measurement problem.

Evaluation of a continuous A-centrifugal at Darnall

Background

Continuous centrifugation of high grade massecuites is not a new concept but has not been widely implemented in raw or refined sugar processing due to unacceptably high levels of crystal breakage, high purity rise, high sugar moisture and lump formation. Recently, several companies claim to have reduced the above problems to the extent that high grade continuous centrifugals now offer an economically feasible alternative to batch machines. The economic advantages are mainly due to reduced maintenance costs, lower capital cost and reduced operator attention required. In order to evaluate this emerging technology, Tongaat-Hulett decided to install a prototype continuous A-centrifugal at Darnall Mill.

Installation details

The continuous A-centrifugal was installed parallel to the existing bank of batch A-centrifugals but with a separate feed line direct from the final A-crystalliser. Sugar from the continuous A-centrifugal was discharged directly into the existing A-sugar screw and was mixed with the product from the batch A-centrifugals. Molasses from the continuous A-centrifugal was discharged into a separate molasses gutter to allow flow rate to be measured.

The continuous A-centrifugal was supplied with its own programmable logic controller (PLC) and 'touch screen' control panel. Variables able to be controlled were massecuite flow rate (based on motor current), centrifugal speed and wash water rates.

Molasses flow measurement

Molasses flow rate was measured by diverting the flow from the continuous A-centrifugal molasses gutter into a 200 litre tank supported on an electronic mass balance. The outlet, located at the base of the tank, was connected to the molasses pump via a flexible hose so as to minimise external forces that would otherwise have been imposed on the tank by the pump connection. High and low level conductivity probes in the tank were installed to start and stop the pump to achieve batch filling and emptying of the tank. The electronic balance was connected to a computer via an RS232 connection allowing mass and corresponding time information to be continuously captured and recorded on a computer disk. Information on the rate of filling of the tank for specified periods could be obtained from the stored data and hence accurate mass flow rates could be determined.

Test procedures

The purpose of the investigation was to evaluate the performance of the continuous A-centrifugal with regard to *capacity*, *sugar quality* and *molasses losses*. Capacity was quoted in terms of massecuite throughput rate, while both sugar quality and molasses losses would be expected to vary as a function of massecuite rate. Hence it was essential to determine the massecuite flow accurately to evaluate the performance of the machine.

An example of a set of tests would be investigation of the effect of varying massecuite throughput rate on sugar and molasses quality for fixed steam addition, massecuite quality, wash water rates and wash position. Each test would require analyses of massecuite, massecuite nutsch, molasses and sugar in order to observe the effect of a particular variable on the quality and composition of the product streams, and to solve mass balances for massecuite flow rate determination.

Massecuite flow rate determination

Due to the practical difficulties and cost associated with measuring massecuite and sugar flow rate directly, it was decided to measure *wash water* and *molasses* flow rates and to determine *massecuite* and *sugar rates* by overall and component mass balances on the centrifugal. Some of the balances which can be used to determine massecuite flow rate are presented in Appendix 1.

However, the mass balance problem was over-specified, due to the number of measurements and analyses available, resulting in there being several solution methods to the problem. When applied to actual trial data, the massecuite flow rate determined by the various conventional mass balances differed by up to 25%. This resulted in significant uncertainty when quoting centrifugal capacity. Reasons for disagreement between the balances, and hence apparent violation of the conservation laws, are that:

- the simplifying assumptions necessary for each mass balance introduce a degree of error which is different for each component balance
- the individual variables are subject to random analytical and measurement error which differ in magnitude for different analyses and instruments.

It was this uncertainty in the estimation of the massecuite flow, because of the known limitations of using conventional mass balance techniques, that prompted the investigation into a better method.

Theory of 'reconciliation of process flows'

The problem of reconciling the inconsistencies in process measurements when evaluated in terms of mass balances has been addressed by a number of authors as summarised by Crowe (1988b) and by Howat in Perry and Green (1997). Much of this work appears to have a strong academic rather than practical bias and to understand the theory requires a familiarity with matrix algebra, multivariate statistics, calculus and optimisation techniques, making it not easily accessible to the average sugar technologist.

The theory is further complicated by the distinction of problems into two different types, viz. linear and nonlinear (Crowe, *et al* 1983; Crowe, 1986). In this context, problems are only linear if both the concentration and the flow rate of a stream are known. A limitation to solving only linear problems would thus be a severe restriction on the usefulness of the technique of reconciliation, making the more advanced techniques for nonlinear problems essential.

Despite the complexity of the mathematics, the principles on which the reconciliation of process flow rates are based can be stated quite simply as follows:

a) Identify and discard any measurements with gross errors.

b) Create an adjusted set of measurements which:

- meets the requirements of a full mass balance
- takes into account the known accuracies of the measurements (i.e. less accurate measurements are adjusted more than the fairly accurate measurements)
- are optimal in terms of making the minimum adjustments to the measurements.

The issue of detecting gross errors although closely allied, is a subject on its own (Crowe, 1988a) and will not be addressed directly here.

There will be an infinite number of sets of adjusted measurements which will meet the requirements of full mass balance, and to select the optimum set, the sum of squares of the adjustments must be minimised. To take account of the known accuracies of the measurements, each squared adjustment must be multiplied by a weighting factor which has been shown to be the inverse of the variance, σ^2, of the measurement. Even approximate values are adequate (Beckman, 1982) and variances can be estimated from the simpler concept of a confidence interval (Kneile, 1995). This addresses the issue of allowing larger adjustments to be made to less accurate data. For example brix measurements with a confidence interval of ±0,45 percentage units should be adjusted less than molasses flow measurements with a confidence interval of ±5% in the process of achieving a set of adjusted data which meets the requirements of a full mass balance.

This reconciliation problem has been summarised mathematically by Beckman (1982) as detailed in Appendix 2.

Expressed in its mathematical form, the problem is termed a constrained optimisation (maximisation or minimisation). In general there are three methods of solving this type of problem (Boas, 1966), viz. elimination, implicit differentiation or the use of Lagrange multipliers. Beckman (1982) has used the technique of elimination in his approach to the reconciliation of process data whilst others (Kneile, 1995; Crowe, *et al.* 1983 and Crowe, 1986) have used Lagrange multipliers. Despite the significant algebraic effort of these approaches, iterative numerical methods are still required by the method of Beckman (1982) and the nonlinear case of Crowe (1986).

Given the complexity of these methods, the question arises as to whether a simpler numerical technique, using the nonlinear optimising capabilities of a modern spreadsheet, can be devised.

A numerical technique for the reconciliation of process flows on a spreadsheet

Modern computer spreadsheets have the capabilities to perform nonlinear optimisation. The Corel Quattro Pro for Windows spreadsheet (versions 6 and 8), which was used in this work, provides such a function named 'Optimizer'. The user need only identify the cell which is to be maximised or minimised and indicate which cells are to be altered to achieve this optimisation. There are also a number of convergence parameters for the optimisation which can be altered to improve the speed and accuracy of the optimisation if desired. The 'Optimizer' function also has the ability to handle constraints if necessary.

The spreadsheet documentation provides limited information on the mathematical methods used to achieve the nonlinear optimisation. In particular, there is no indication of how the constraints are handled. The user thus needs to treat the 'Optimizer' function much like a 'black box' which will give the correct output if the input is correctly specified.

As part of this work, a technique was developed which provides a simple way of handling constraints within the standard nonlinear optimisation without requiring the spreadsheet's ability to handle constraints. This 'engineering' method of handling constraints is simply to add the weighted sum of squares of the adjustments (described above) to the weighted sum of squares of the imbalances in the constraint equations (which should be zero). Minimisation of this new, augmented, sum of squares function will thus force the constraints to be met to an accuracy defined by the weighting function. Appendix 2 shows how this concept can be expressed in the mathematical format used by Beckman (1982).

Although this method of handling constraints is not mathematically rigorous, it meets the engineering requirement of being 'good enough for all practical purposes'. For example, the user can decide whether to force the overall mass balance to converge to within 1 kg/s or 1 g/s, whichever is accurate enough in terms of the precision and accuracy of the measurements being used.

This 'engineering method' is much simpler than the rigorous mathematical methods used by Beckman (1982), Kneile (1995) and Crowe (1986). It also has an advantage over using the built-in constraint handling of the Quattro spreadsheet in that the way that the constraints are handled is more transparent to the user and can be manipulated if necessary by altering the weighting function. Specifically, the user should select the smallest weighting function necessary to force the constraints to converge to the required accuracy. Large weighting functions will force the constraints to converge but will make the sum of squares function insensitive to the adjustments in the measurements, achieving poor, or no, convergence in this respect.

Application of the numerical reconciliation of process flows (NRPF) technique to a continuous A-centrifugal

The numerical reconciliation of process flows (NRPF) technique was developed for the continuous A-centrifugal trials due to uncertainty resulting from the wide range of massecuite flow rates obtained from the different conventional mass balances (Appendix 1) using the same measured and analytical data.

Prior to applying the NRPF technique to normal test data, the accuracy and robustness of the technique was first evaluated by the following methods:

- The NRPF and conventional mass balance solutions were compared against a simulated set of ideal data which satisfied the material balance constraints for a massecuite flow rate of 30 t/h.
- The NRPF technique was compared against the conventional mass balances using six simulated data sets containing known random errors added to ideal data.
- The NRPF and conventional mass balance solutions were compared against solutions from an overall mass balance which included measurement of sugar flow rate (which would not be available in normal test work).

Application of the NRPF Spreadsheet

The application of the NRPF spreadsheet program for flow rate reconciliation is relatively simple and the method could be applied universally to any unit operation where steady state mass balances apply. The program adjusts the measured and analytical data to satisfy the overall mass balance, dry solids balance and pol balance for the continuous A-centrifugal trials.

Balances:

Overall: $\mathrm{Tons}_{M/C}+\mathrm{Tons}_{H2O}-\mathrm{Tons}_{sug}-\mathrm{Tons}_{mol}=0$ Constraint (2)
Pol: $\mathrm{Pol}_{M/C}T_{M/C} - \mathrm{Pol}_{sug}T_{sug} - \mathrm{Pol}_{mol.}T_{mol}=0$ Constraint (3)
Dry Solids: $\mathrm{DS}_{M/C}T_{M/C} - \mathrm{DS}_{sug}T_{sug} - \mathrm{DS}_{mol}T_{mol}=0$ Constraint (3)

Note: Dry solids were used instead of brix due to the errors associated with the optical nature of brix measurement. However, brix could just as well have been used. An empirical relationship derived within Tongaat-Hulett Sugar ([1]private communication) was used to estimate 'dry solids' from brix and pol measurements. The relationship is:

$$\text{Dry Solids} = \text{Brix} * (1 - 0{,}00066*(\text{Brix} - \text{Pol})).$$

A Quattro Pro spreadsheet (Table 1) was designed to apply the NRPF technique to the continuous A-centrifugal. The optimizer (*Tools-Numeric Tools-Optimizer* menu option) is set up to adjust the *Measured Values (G_j)* (Spreadsheet cells D4 .. D13) in order to minimise the *Total Weighted Squared*

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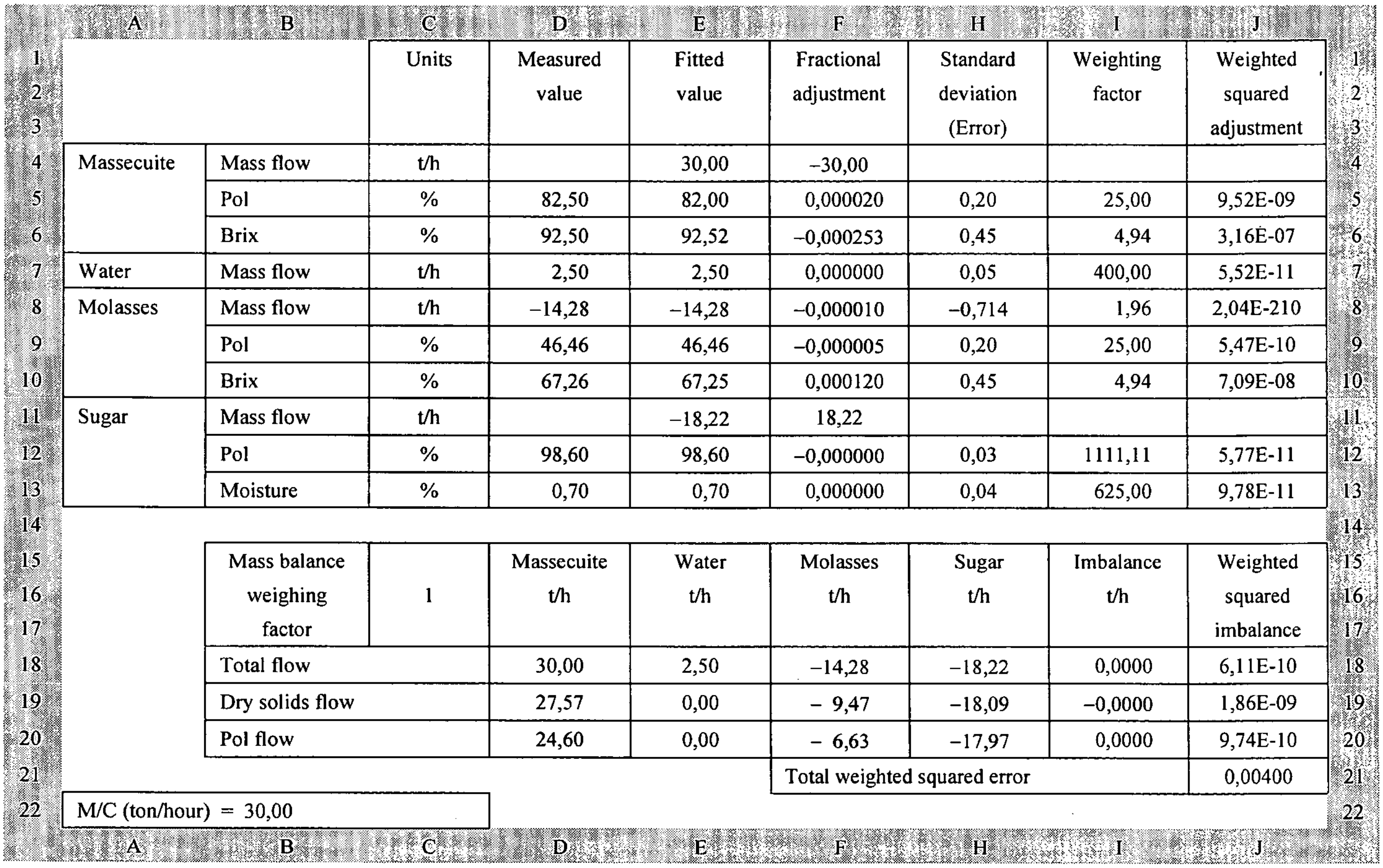
Error (SSQ2, per Eq. (5)) (Spreadsheet cell J21). The *Weighting Factors (WF_j and Wx_{ij})* (Spreadsheet cells I4..I13) were determined from the *Standard Deviation* values (Spreadsheet cells H4..H13) of the various analyses and measurements. The standard deviations are estimated from the confidence intervals, namely:

Brix analytical error = ±0,45%
Pol analytical error = ±0,20%
Molasses flow error = ±5% of actual measurement
Water flow error = ±2% of actual measurement.

Thus the weighting factors reflect these confidence intervals, with large factors indicating high confidence in the data.

The *Total Weighted Squared Error (SSQ2)* (Spreadsheet cell J21) comprises the sum of the *Weighted Squared Adjustments (SSQ1, per Eq. (1))* (Spreadsheet cells J4..J13) and the *Weighted Squared Imbalance* of each mass balance (Spreadsheet cells J18..J20), per Eq. (5). In order to ensure that the material balance constraints were met, a *Mass Balance Weighting Factor (WB)* of 1 (Spreadsheet cell C16) was applied to each of the squared mass balances. This can be varied by the user to achieve the required convergence of the balances on the adjusted data. As mentioned previously, this value should be the minimum necessary to achieve the required convergence.

Table 1. Example of the NRPF spreadsheet using an ideal data set with a massecuite flow rate of 30 t/h.



		Units	Measured value	Fitted value	Fractional adjustment	Standard deviation (Error)	Weighting factor	Weighted squared adjustment
Massecuite	Mass flow	t/h		30,00	–30,00			
	Pol	%	82,50	82,00	0,000020	0,20	25,00	9,52E-09
	Brix	%	92,50	92,52	–0,000253	0,45	4,94	3,16E-07
Water	Mass flow	t/h	2,50	2,50	0,000000	0,05	400,00	5,52E-11
Molasses	Mass flow	t/h	–14,28	–14,28	–0,000010	–0,714	1,96	2,04E-210
	Pol	%	46,46	46,46	–0,000005	0,20	25,00	5,47E-10
	Brix	%	67,26	67,25	0,000120	0,45	4,94	7,09E-08
Sugar	Mass flow	t/h		–18,22	18,22			
	Pol	%	98,60	98,60	–0,000000	0,03	1111,11	5,77E-11
	Moisture	%	0,70	0,70	0,000000	0,04	625,00	9,78E-11

Mass balance weighing factor	1	Massecuite t/h	Water t/h	Molasses t/h	Sugar t/h	Imbalance t/h	Weighted squared imbalance
Total flow		30,00	2,50	–14,28	–18,22	0,0000	6,11E-10
Dry solids flow		27,57	0,00	– 9,47	–18,09	–0,0000	1,86E-09
Pol flow		24,60	0,00	– 6,63	–17,97	0,0000	9,74E-10
				Total weighted squared error			0,00400

M/C (ton/hour) = 30,00

Comparison of the NRPF technique with conventional mass balances using simulated ideal data

The purpose of comparing the NRPF technique and the conventional balances with a known massecuite flow rate was to select those balances which produced the most accurate results and also to check the relative accuracy of the flow rates with the conventional balance flow rates.

A set of simulated ideal data satisfying the *overall*, *pol* and *dry solids* material balance constraints, was generated based on a massecuite flow rate of 30 ton/hour (Appendix 3, Table 5). Molasses brix was determined from dry solids using the correlation described above and hence the brix balance is not completely satisfied and has a maximum imbalance (error) of approximately 0,5%.

The ideal data set was used to calculate massecuite flows using the conventional mass balances and the NRPF technique. The results are presented in Table 2.

Five of the 11 solutions above have absolute errors of less than 1%. This represents the difference between the calculated massecuite flow rate and the ideal flow of 30 t/h. A further three balances have solutions with absolute errors ranging from 1,78 to 4,03%, while the remaining three balances all have errors greater than 5%. The reasons for any deviation from the ideal massecuite flow of 30 t/h are due to the simplifying assumptions made in solving each of the balances. The NRPF solution ranked third in terms of accuracy and had an absolute error of only 0,07%. However, at this very low level of error the relative ranking is not significant and is probably affected by round-off errors.

Based on the above comparison of the various mass balances, using ideal data, it was decided to investigate further only those which resulted in solutions with an absolute error of less 1%, i.e. the balances which were greater than 99% accurate. These balances are ranked 1 to 5 in Table 2 and comprised four conventional mass balances and the NRPF technique.

It is interesting to note that three of the best four conventional balances were all based on data which were not directly analysed for, namely, non-pol or non-crystal. This is most likely due to the fact that non-pol (%) and non-crystal (%) were determined by difference of pol and moisture (100-brix) from 100. This could have an 'averaging' effect on the errors resulting from the simplifying assumptions in the calculations.

Table 2. Comparison of mass balances using an ideal data set.

Conventional mass balances	M/C flow (tons/h)	Absolute error (%)	Ranking
Balance A1	30,78	2,59	7
Balance A2	30,01	0,03	2
Balance B1	26,48	11,72	11
Balance B2	27,78	7,40	10
Balance C1	28,29	5,71	9
Balance C2	28,29	4,03	8
Balance D1	29,47	1,78	6
Balance D2	30,00	0,00	1
Balance E1	29,73	0,88	5
Balance E2	29,86	0,47	4
NRPF M/C flow rate	29,98	0,07	3
Mean	29,20		
Standard deviation	0,99		

Note: Absolute error is the % difference between the calculated M/C flow rate and the ideal flow rate of 30 tons/hour.

Comparison of the NRPF technique with conventional mass balances using simulated data with known random errors

If the degree of accuracy of measured data in a real situation was known, it would be a trivial task to select the mass balance which would provide the 'best' solution. However, in the case of the continuous A-centrifugal trial there will be random and unknown errors in the measured data. It was therefore decided to investigate how robust each of the accepted alternative calculation methods were when used on simulated data with known random errors.

In Appendix 4, six sets of simulated data containing normally distributed measurement errors were calculated from the ideal data of Appendix 3, and are shown in Table 6. Massecuite flow rates were then calculated (Table 7) using the accepted balances and the results were compared. The six random data sets as well as detailed solutions are presented in Appendix 4. A summary of the results is presented in Table 3.

In Table 3, the mean values represent the average massecuite flow rate calculated over the six random data sets while the standard deviation indicates the variation of data about the mean. The absolute mean error is the difference between the massecuite flow rate calculated by a particular type of balance for the ideal data set (i.e. without errors), and the mean massecuite flow rate of the six data sets containing random errors. Each of the balance types were assigned rankings based on absolute mean errors. Previous rankings determined on ideal data are repeated for comparison.

It is evident from the rankings that the two most robust massecuite flow determination methods, both in terms of absolute mean error and standard deviation, are the NRPF technique and Balance A2 (dry solids balance using molasses and wash water rates). However all the balance types selected show good agreement with massecuite flows calculated for the ideal data.

Comparison of the NRPF technique and conventional mass balances with an overall balance using actual experimental data

In order to confirm the accuracy of the conventional mass balances and the NRPF technique when applied to real data, sugar flow, which would not be available during normal tests to evaluate the centrifugal, was measured in two special tests.

Table 3. Summary of comparison between mass balances using ideal data with known random errors.

Conventional mass balances	Ideal data		Six data sets containing random errors			
	M/C flow (t/h)	Ranking	Mean	Standard deviation	Absolute mean error (%)	Ranking
Balance A2	30,01	2	30,39	1,37	1,26	1
Balance D2	30,00	1	29,09	2,12	3,03	5
Balance E1	29,73	5	28,98	1,74	2,53	4
Balance E2	29,86	4	29,11	1,76	2,51	3
NRPF M/C flow rate	29,98	3	29,45	1,34	1,76	2
Mean	29,92					
Standard deviation	0,11					

Note: Absolute mean error is the % difference between the mean M/C flow rate, determined from the six random data sets, and the ideal data flow rate calculated by that particular balance.

This allowed an overall mass balance to be performed about the centrifugal enabling massecuite flow rate to be calculated.

$$\text{Tons}_{M/C} = \text{Tons}_{mol} + \text{Tons}_{sug} - \text{Tons}_{H2O}.$$

Overall mass balance does not require any laboratory analyses and hence eliminates any random analytical error. Sugar flow rate from the continuous A-centrifugal was determined by using a sugar servo-balance located immediately after the dryer at Darnall and stopping all the batch centrifugals. The servo balance sums batches of about 500 kg and is accurate to ±5 kg per tip. Hence, a 1% accuracy was assumed for reconciliation purposes.

The two runs were performed at different massecuite feed rates over a period of 30 minutes each. Molasses and sugar samples were taken and molasses flow rate was checked at the start, middle and end of each run. This allowed the massecuite flow rate to be calculated by the conventional balances and the NRPF technique. These were then compared with the *overall balance* flow rates in Table 4.

Table 4. Comparison of mass balance types with an overall mass balance using actual experimental data (with extra measurements).

Conventional balances (flow = t/h)	Run 1		Run 2		Average error (%)	Ranking
	M/C flow	Error (%)	M/C flow	Error (%)		
Overall balance	18,35		26,89			
Balance A2	19,28	5,07	26,20	2,57	3,82	2
Balance D2	17,31	5,67	25,51	5,13	5,40	3
Balance E1	17,68	3,65	24,49	8,93	6,29	5
Balance E2	17,78	3,11	24,62	8,44	5,77	4
NRPF M/C flow rate	18,18	0,93	25,85	3,87	2,40	1

The reconciled flow rates using the NRPF method resulted in the lowest average error of 2,4% from the massecuite flow rates determined using the overall balance. Each mass balance has been ranked according to the average errors. Errors for the conventional mass balances range from 3,82 to 5,77%.

The above results confirm the robustness and hence the reliability of the NRPF technique for application to actual plant data.

Reconciliation of actual data from the continuous A-centrifugal trials

The NRPF technique has demonstrated its accuracy and robustness in its application to simulated ideal data, simulated data with known random errors and actual plant data with extra measurements. Given this 'proof' in application and its sound theoretical basis, it was selected as the best method for estimating massecuite flow in evaluating the continuous A-centrifugal. It is of interest to compare the results of this method with what would have been estimated if the more conventional methods had been used.

The data from a trial comprising six individual experimental runs were used to calculate massecuite flow rates. Raw experimental data is presented as Table 8 in Appendix 5. The aim of this particular trial was to investigate the effect of increasing massecuite throughput on sugar and molasses quality. The relative percentage difference between the conventional balance massecuite flows and corresponding NRPF flows for the six experiments are presented in Figure 1.

While average differences between massecuite flows determined by each of the accepted conventional mass balances and those determined by the NRPF technique range between 0,39 and 5,31%, the maximum difference is as high as 16,7% (Balance A2, Experiment 5 in Figure 1). This indicates the significant level of error which could result from randomly selecting a particular conventional balance and ignoring some measurements.

Figure 1 also gives an indication of the relative bias of the conventional balances relative to the NRPF technique. Balance A2 flow rates have a positive offset increasing at higher flow rates. Balance D2 flow rates have a negative offset increasing (-ve) at higher flow rates. Balance E1 and E2 are very similar with positive offsets at low flow rates and increasingly negative offsets at higher flow rates.

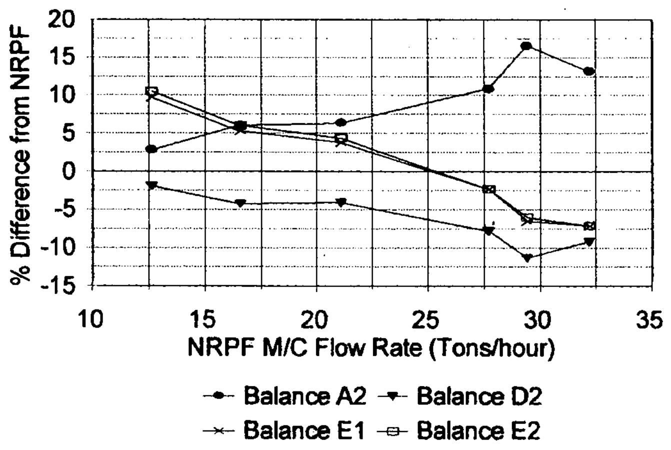


Figure 1. Comparison of mass balance types using actual plant data from the continuous A-centrifugal.

Conclusions

Determination of massecuite flow rates, using the various possible conventional mass balances on a continuous A-centrifugal, resulted in a significant degree of uncertainty due to the differing solutions obtained using the same measured and analytical data. To overcome this, a numerical method, with a sound theoretical base, was developed for the reconciliation of the process flows.

Before applying this technique to the evaluation of the performance of a continuous A-centrifugal, the technique was evaluated as follows:

- The accuracy of the NRPF techniques was tested against conventional mass balances using a simulated ideal data set with a known flow rate and proved to be 99,98 % accurate.
- The robustness of the NRPF technique was tested against simulated ideal data containing random errors and proved to be as robust as the best of the conventional mass balances.
- The NRPF technique was tested against conventional mass balances using actual plant data with extra measurements and compared better with the overall mass balance massecuite flow rate than any of the conventional balances.

The NRPF technique is easily applied to actual experimental data and provides a more reliable estimate of massecuite flow. The technique has been shown to give results which are at times significantly different from more conventional mass balance methods.

The numerical reconciliation of process flows technique is simple and can be universally applied to any unit operation where steady state mass balances apply.

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APPENDIX 1

Mass balances for determining the massecuite feed rate to a continuous centrifugal.

Balance A1 : Brix balance using molasses and wash water flow rates

$$\text{Tons}_{M/C} = \frac{\text{Tons}_{mol}\left(1 - \dfrac{\text{Bx}_{mol}}{(100 - \text{moisture})}\right) - \text{Tons}_{H_2O}}{\left(1 - \dfrac{\text{Bx}_{M/C}}{(100 - \text{moisture})}\right)} \qquad (1)$$

Balance B1 : Combined brix and non-pol solids balance using wash water rate

$$\text{Tons}_{M/C} = \frac{\text{Tons}_{H_2O}}{\left(\dfrac{\text{NP}\,\%_{M/C}}{\text{NP}\,\%_{mol}}\right)\left(1 - \dfrac{\text{Bx}_{mol}}{100 - \text{moisture}}\right) - \left(1 - \dfrac{\text{Bx}_{M/C}}{100 - \text{moisture}}\right)} \qquad (2)$$

Balance C1 : Non-pol solids balance using molasses rate

$$\text{Tons}_{M/C} = \text{Tons}_{mol}\left(\frac{\text{NP}\,\%_{mol}}{\text{NP}\,\%_{M/C}}\right) \qquad (3)$$

Balance D1 : Non-pol solids balance including non-pol in sugar

$$\text{Tons}_{M/C} = \frac{\text{Tons}_{H_2O}(\text{Bx}_{sug} - \text{Pol}_{sug}) + \text{Tons}_{mol}(\text{Bx}_{mol} - \text{Pol}_{mol} - \text{Bxsubsug} + \text{Pol}_{sug})}{(\text{Bx}_{M/C} - \text{Pol}_{M/C} - \text{Bx}_{sug} + \text{Pol}_{sug})} \qquad (4)$$

Balance E1 : Non-crystal balance

$$\text{Tons}_{M/C} = \frac{\text{Tons}_{mol}(1 - \text{Bx}_{mol}) - \text{Tons}_{H_2O}}{\left(1 - \dfrac{\text{CC}}{100}\right)(1 - \text{Bx}_{nutsch})} \qquad (5)$$

The above balance equations can be converted to dry solids balances rather than brix balances by replacing the brix terms with an empirical relationship developed within Tongaat-Hulett Sugar (Balances A2 to E2 respectively). The relationship is:

Dry Solids (DS) = Brix (1 – 0,00066 (Brix – Pol)).

APPENDIX 2.
Mathematics of process flow reconciliation.

Beckman (1982) has summarised the reconciliation of process flow problem mathematically as minimising the weighted sum of squares function, *SSQ*1, which is given by:

$$SSQ1=\sum_{j=1}^{M}\frac{WF_j}{G_j^2}\left(G_j-F_j\right)^2+\sum_{j=1}^{M}\sum_{i=1}^{N}\frac{Wx_{ji}}{y_{ji}^2}\left(y_{ji}-x_{ji}\right)^2$$

Where:

$SSQ1$ = Sum of squares function to be minimised
$WF_j = 1/\sigma_{Fj}^2 =$ Weighting factor for stream j flow rate
$Wx_{ji} = 1/\sigma_{xij}^2 =$ Weighting factor for stream j composition
G_j = Measured flow rate of stream j
y_{ji} = Measured composition of component i in stream j
F_j = Adjusted flow rate of stream j
x_{ji} = Adjusted composition of component i in stream j
M = Total number of flow streams
N = Total number of components
σ = Standard deviation of measurement
σ^2 = Variance of measurement.

Subject to the following constraints:

$$\sum_{j=1}^{M}F_j=0$$

i.e. the sum of the mass flows in (taken as positive) equals the sum of the mass flows out (taken as negative).

$$\sum_{j=1}^{M}F_jx_{ji}=0 \qquad 1\leq I\leq N$$

i.e. for each .i-th. component of all N components the sum of the mass flows in equals the sum of the mass flows out.

$$\sum_{i=S(j)}^{N}x_{ji}=1 \qquad 1\leq j\leq M$$

where *S(j)* is the index of the first non-zero valued component in stream *j*.

i.e. the adjusted compositions of all the components in each stream must sum to unity (with the adjusted values of all compositions measured as zero being forced to zero).

Kneile (1995) described how the simpler concept of a confidence interval of ±*a* can be used to estimate the variance, σ^2, as:

$$\sigma^2=\left(\frac{a}{1{,}96}\right)^2$$

by assuming that ±*a* is the 95% confidence interval of a normal probability distribution. Generally, for the full mathematical analysis of the problem, it is assumed that the measurement errors are independent of each other.

The numerical technique for dealing with the constraints using conventional, unconstrained, optimisation can be expressed mathematically in the format used by Beckman (1982) as:

$$SSQ2=SSQ1+WB\left(\left(\sum_{j=1}^{M}F_j\right)^2+\sum_{i=1}^{N}\left(\sum_{j=1}^{M}F_jx_{ji}\right)^2\right)$$

Where:

$SSQ2$ = augmented sum of squares function to be minimised
WB = weighting factor for the squared imbalance of constraints

and the rest of the variables are as previously defined.

The constraint for forcing all the individual component fractions of a stream to sum to unity can be neglected in most sugar factory applications as in the equation above. This is because there is usually a pseudo component called non-pol or non-sucrose which is never measured but is simply calculated by difference. The component fractions can thus be forced to sum to unity by leaving non-pol out of the optimisation and simply calculating it by difference once the optimisation has been done.

The mathematical descriptions of the reconciliation problem can probably be more easily understood by referring to the spreadsheet example given in Figure 1 where the variables and subscripts can be interpreted as follows.

Subscript 'j' refers to the different streams with

j = 1	massecuite
j = 2	water
j = 3	molasses
j = 4	sugar.

Subscript 'i' refers to the different constituents of a stream

i = 1	pol
i = 2	brix or (100-moisture).

Thus, for example

G_2	is the measured mass flow of water
y_{32}	is the measured brix of molasses
F_2	is the adjusted mass flow of water
x_{32}	is the adjusted brix of molasses
WF_3	is the weighting factor for the adjustments to the mass flow of molasses
Wx_{32}	is the weighting factor for the adjustments to the brix of molasses.

APPENDIX 3.

Table 5. Ideal data generation based on fixed massecuite flow rate.

FEED to continuous centrifugal	
Massequite	
Assume flow rate (t/h)	30,00
Assume massecuite brix %	92,50
Assume massecuite Pol %	82,00
Massecuite DS %	91,86
Massecuite purity %	88,65
Crystal content %	60,61
Crystal flow in M/C (t/h)	18,18

Nutsch	
Assume Nutsch brix %	82,00
Nutsch DS %	80,54
Assume Nutsch Pol %	55,00
Nutsch purity %	67,07

Water	
Assume flow rate (t/h)	2,50
Wash % M/C	8,33

PRODUCT from continuous centrifugal	
Sugar	
Assume 'wet' Pol % (ex centrifugal)	98,60
Assume moisture % (ex centrifugal)	0,70
Sugar brix %	99,30
Sugar DS %	99,25

Crystal balance	
Assume crystal loss %	3,00
Hence crystal flow in sugar (t/h)	17,64
Assume sugar Nutsch purity % (= M/C Nutsch purity + 5 units)	72,07
Sugar crystal content %	96,79
Hence sugar flow rate (t/h)	18,22

Molasses properties	
Molasses brix %	67,26
Molasses DS %	66,34
Molasses Pol %	46,46
Molasses purity %	69,07
Purity rise %	2,98

Balance check	M/C	Water	Molasses	Sugar	Imbalance
Overall mass balance	30,00	2,50	14,28	18,22	0,0000
DS balance	27,56	0,00	9,47	18,09	0,0000
Pol balance	24,60	0,00	6,63	17,97	0,0000

APPENDIX 4.

Random data sets and mass balance solutions based on ideal data.

Table 6. Simulated ideal data with random known errors (actual massecuite flow = 30 t/h).

	Ideal data	Error	Standard deviation	Normal distribution of random data with ideal data as mean value					
				Data 1	Data 2	Data 3	Data 4	Data 5	Data 6
Moisture flow rate (t/h)	14,28	5%	0,71	13,80	14,55	13,60	12,64	14,80	14,14
Wash water rate (t/h)	2,60	2%	0,05	2,56	2,52	2,51	2,54	2,50	2,55
Massecuite Pol	82,00	0,20	0,20	81,97	82,01	82,06	82,20	82,16	81,68
Massecuite brix	92,60	0,45	0,45	91,97	92,95	92,64	92,80	91,94	92,36
Nutsch Pol	66,00	0,20	0,20	55,24	55,12	54,66	55,20	55,03	55,03
Nutsch brix	82,00	0,45	0,45	81,89	81,70	81,92	81,73	82,15	82,89
Molasses Pol	46,46	0,20	0,20	46,31	46,51	46,35	46,55	46,68	46,56
Molasses brix	67,26	0,45	0,45	67,08	67,41	67,25	66,76	66,64	66,80
Wet sugar Pol (ex centrifugal)	98,60	0,03	0,03	98,59	98,61	98,61	98,58	98,55	98,61
Sugar moisture (ex centrifugal)	0,70	0,04	0,04	0,67	0,75	0,71	0,77	0,67	0,70
Calculated M/C dry solids	91,86			91,36	92,28	91,99	92,15	91,34	91,71
Calculated Nutsch dry solids	80,54			80,45	80,27	80,45	80,30	80,68	81,36
Calculated moisture dry solids	66,34			66,16	66,48	66,32	65,87	65,76	65,90
Calculated sugar dry solids	99,25			99,28	99,21	99,24	99,19	99,27	99,25

APPENDIX 4 (continued)

Table 7. Massecuite flow rate determination for simulated ideal data with random known errors.

Conventional mass balances	M/C flow (t/h)	Random data 1	Random data 2	Random data 3	Random data 4	Random data 5	Random data 6	Mean	Standard deviation
Balance A1	30,78	25,86	33,77	28,11	24,67	31,86	29,77	29,01	3,19
Balance A2	30,01	28,38	31,65	30,62	32,36	29,06	30,25	30,39	1,37
Balance B1	26,48	31,20	24,17	26,03	23,76	28,82	24,77	26,46	2,70
Balance B2	27,78	32,84	25,30	27,30	24,87	30,29	25,95	27,76	2,89
Balance C1	28,29	28,66	27,80	26,88	24,10	30,22	26,79	27,41	1,88
Balance C2	28,79	29,17	28,30	27,36	24,54	30,76	27,27	27,90	1,91
Balance D1	29,47	30,07	28,79	27,96	25,02	31,77	27,83	28,57	2,09
Balance D2	30,00	30,61	29,31	28,46	25,48	32,34	28,34	29,09	2,12
Balance E1	29,73	29,17	29,52	28,53	25,91	31,86	28,91	28,98	1,74
Balance E2	29,86	29,29	29,63	28,65	26,02	32,01	29,06	29,11	1,76
NRPF M/C flow rate	29,98	28,17	30,61	17,97	29,20	31,76	29,00	24,62	11,09

APPENDIX 5.

Table 8. Raw experimental data.

Exp No.	Moisture flow (kg/s)	Water (kg/s)	Massecuite				M/C Xtal Cont	Massecuite Nutsch			
			Brix	DS	Pol	Purity		Brix	DS	Pol	Purity
1	2,22	0,549	91,75	90,99	79,27	86,40	56,47	82,55	80,96	53,35	64,63
2	2,68	0,549	91,75	90,99	79,27	86,40	56,47	82,55	80,96	53,35	64,63
3	3,22	0,549	91,75	90,99	79,27	86,40	56,47	82,55	80,96	53,35	64,63
4	3,90	0,549	91,75	90,99	79,27	86,40	56,47	82,55	80,96	53,35	64,63
5	4,02	0,549	91,75	90,99	79,27	86,40	56,47	82,55	80,96	53,35	64,63
6	4,29	0,549	91,75	90,99	79,27	86,40	56,47	82,55	80,96	53,35	64,63

Note: Measured and analytical data are presented in columns 2, 3, 4, 6, 9 and 11.

Exp No.	Molasses				Purity rise	Sugar			
	Brix	DS	Pol	Purity		Pol	Moisture	DS	Corr Pol
1	62,25	61,49	43,75	70,28	5,65	98,48	0,95	99,01	99,36
2	64,90	64,06	45,25	69,72	5,09	98,58	0,87	99,09	99,38
3	67,85	66,91	46,90	69,12	4,49	98,26	1,23	98,74	99,42
4	68,85	67,87	47,25	68,63	4,00	98,06	1,18	98,77	99,18
5	68,25	67,28	46,75	68,50	3,87	97,89	1,46	98,50	99,28
6	69,20	68,19	47,00	67,92	3,29	97,55	1,43	98,50	98,93

Note: Measured and analytical data are presented in columns 2, 4, 7 and 9.

The duration of each experiment run was four minutes, with one minute between runs.

DS = Dry solids