REFEREED PAPER

MATLAB® modelling of a sugar mill: model development and validation

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Abstract

The Sugar Milling Research Institute NPC in Durban, in collaboration with the University of KwaZulu-Natal, is undertaking broad techno-economic modelling of the sugarcane biorefinery as a basis for selecting products and processes with the highest potential for successful implementation. A case study modelling of pre-selected plant configurations involving mass and energy balances of individual units constituting a generic sugar mill as basis for a biorefinery was adopted.

The presented study reports on a MATLAB® model of a raw sugar mill. A plant configuration with mud filtration, five-effect evaporation and a three-boiling partial remelt scheme for the boiling house was selected. Special emphasis was placed on the method of boiling house modelling. The MATLAB® model was successfully verified against calculation results obtained from the Sugars™ simulation program for the same input data. The model validation task included over 50 factory performance indicators taken from the 90th Annual Review of the Milling Season in Southern Africa (2014-2015) (Smith et al., 2015). An optimal set of model parameters that produced a data fit within the mean standard deviation of factory figures from several South African mills, was obtained. A new solubility coefficient equation, specific to sugar streams encountered in the South African sugar industry, was also proposed.

Keywords: sugar mill, model, validation, factory performance, biorefinery.

Introduction

The mathematical model of a typical South African sugar mill is the central part of the Biorefinery Techno-Economic Modelling (BRTEM) project undertaken by the Sugar Milling Research Institute NPC (SMRI) and the University of KwaZulu-Natal in Durban. The first phase of the project involved the MATLAB® modelling and simulation of a system consisting of a sugar mill, an ethanol plant and a power cogeneration plant (Starzak & Zizhou, 2015). Model simulations were performed for arbitrarily selected system parameters and operating conditions. The part of the calculation that referred to the operation of the sugar mill was then checked against predictions obtained from the Sugars™ program (Weiss, 2013). Using an equivalent plant model and input data, the comparison showed the models to be in excellent agreement (Starzak & Davis, 2015). Small but practically negligible discrepancies were due to simplifications made in modelling the operation of a few separation units such as the diffuser or the mud vacuum filter. In addition, some of the physical properties were modelled using different empirical correlations, e.g. the boiling point elevation. Nevertheless, that phase of the sugar mill modelling represented only a verification of the proposed model in terms of its formal mathematical correctness. The proper model validation based on actual factory performance data and a determination of the sugar mill operating parameters is the subject of this study.

Although there are several commercially available process simulators that, in principle, can be used to model a sugar mill, such as Chemcad® or ASPEN®, modelling of sugar streams with these programs becomes a challenge due to the very specialised physical property database required. Moreover, neither commercial process simulators nor even the dedicated Sugars™ program are suitable for performing comprehensive model validation tasks. The systematic model validation procedure, where a large number of model parameters must be optimised in order to minimise the deviations of model predictions from observed plant data, can practically be realised only through using a low-level programming language such as MATLAB®. Even though programmatically much more intensive, this computational tool offers more flexibility in terms of modelling thermophysical and thermodynamic properties of the media characterising sugar mill processes as well as more freedom in the parameter optimisation strategies employed.

Sugar mill model development

The sugar mill model was developed with the intention of creating a generic representation of a typical South African mill. A decision was made to choose a process configuration involving a mud filtration step, a five-effect evaporation station and a three-boiling partial remelt scheme for the boiling house. The entire sugar mill model consists of six modular blocks: extraction, clarification and filtration, evaporation, crystallisation, sugar drying and utilities (boiler and cooling tower). With only a few exceptions, the level of detail used in the plant modelling is identical to that offered by the commercial Sugars™ simulation program.

Extraction

The sugar extraction plant model consists of cane knives and a shredder, a diffuser with steam injection, bagasse mills, a steam-injected press water tank and a diffuser heat exchanger. The motive superheated steam is supplied by a low-pressure boiler (31 bar abs). It is used for cane preparation as well as running the bagasse dewatering and drying mills, both represented by a single unit. The exhaust steam is at 2 bar and 121ºC. A pre-specified fixed amount of steam per tonne of cane processed is used in calculations. Bleed steam from evaporators is used to heat the diffuser and the press water tank.

Clarification and Filtration

The clarification and filtration plant model involves the following units: mixed juice tank, primary juice heater, juice-lime blender, secondary juice heater, tertiary juice heater, juice flash tank, clarifier, mud-bagacillo blender and mud vacuum filter. The mixed juice tank collects three streams: draft juice from the diffuser, juice recovered from the vacuum filter and a small amount of sludge from the syrup filter in the evaporation plant. The mixed juice is pumped and heated by evaporator bleed vapours and by exhaust steam in a train of three heat exchangers. After the primary heater, milk of lime is added. The flash tank is used to remove air from the juice by bringing the juice pressure down to atmospheric. The mud from the clarifier is then blended with bagacillo (treated as bagasse) to facilitate the mud filtration process. The filtrate from the mud vacuum filter is recycled back to the mixed juice tank.

Evaporation
The evaporation plant model involves a clarified juice preheater, five evaporators, four condensate flash tanks (starting from 2nd effect), a syrup filter and a barometric condenser. The five effects of the evaporation station are configured in a co-current mode. Exhaust steam from a back-pressure turbo alternator (utilities plant) and the mill turbine (extraction plant), both at 2 bar and 121ºC, is used for juice heating in the preheater and boiling in the first evaporator. Pressures in the individual evaporators were pre-specified at 1.60, 1.25, 0.60, 0.40 and 0.16 bar, being typical values for a quintuple effect evaporator station under South African conditions (Peacock, 2015). A fixed pressure drop of 0.02 bar per effect was assumed to account for hydraulic losses. In addition, the pressure profile includes a provision for a vapour throttle valve (0.15 bar drop) used for brix control, which is common in the South African sugar industry. For a five-effect evaporation station, the syrup brix is controlled by throttling the vapour feeding the third effect vessel. This design "buffer" allows for some spare evaporation driving force in the system to allow for peak flow conditions. Based on the review done in several sugar mills in the region, the following vapour bleeding scheme was adopted as the most representative of the local industry:

- 1st vapour: tertiary mixed juice heater, press water tank, diffuser injection, A-pan, B-pan;
- 2nd vapour: secondary mixed juice heater, diffuser heater, remelter, C-pan;
- 3rd vapour: primary mixed juice heater

A series of flash tanks is used to flash condensates from various parts of the sugar mill and use the resulting vapours for heating in evaporators.

Crystallisation
The crystallisation plant model consists of A, B and C pans; A, B and C crystallisers (A, C – water-cooled, B – air-cooled); A, B and C centrifuges; a remelter heated by steam injection; a B-magma mingler; and a barometric condenser. The implementation of the three-boiling partial remelt scheme is shown in Figure 1. A model of a two-output centrifuge has been adopted from the Sugars™ simulation program (Weiss, 2013) to predict the separation performance of A, B and C centrifuges. A number of stream specifications are required for the proper formulation of the crystallisation plant simulation problem, e.g. brix, temperature and supersaturation of pan massecuites, temperature and supersaturation of crystalliser massecuites, centrifuge operation parameters, etc. The amount of B-magma sent to the A pan is controlled by the requirement that the number of crystals in the magma stream should be equal to that in the stream leaving the pan.

Sugar drying
The proposed model of sugar drying involves a rotary drum dryer and an air heater. A fictitious crystallisation unit is used to account for the effect of sugar crystallisation from the residual syrup accompanying sugar crystals when exposed to high drying temperatures.

Utilities
It is assumed that a low-pressure boiler generates superheated steam at 31 bar and 390ºC. A very simple model of the boiler was adopted from the existing Sugars™ model. It is based on the assumption that a pre-specified amount of bagasse is required and available to generate 1 tonne of superheated steam of a given pressure and temperature. For the selected steam parameters and 51% moisture in bagasse, a reasonable estimate is 0.45 t/t (Rein, 2007). Consequently, modelling of the ash and flue gas streams was not undertaken. Similarly, no

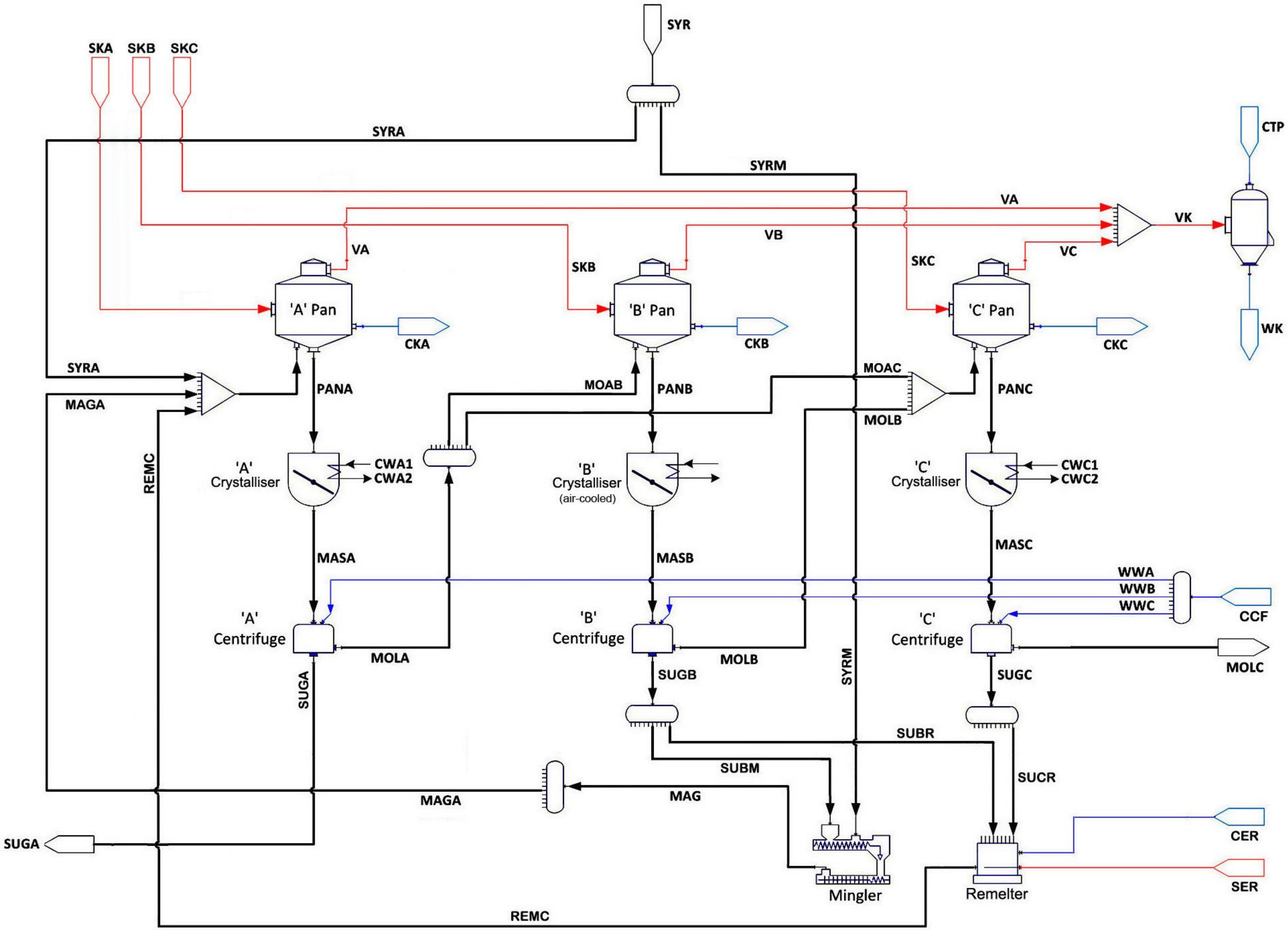


Figure 1. Typical South African boiling-house configuration with a three-boiling partial remelt scheme.

heat recovery from flue gas, such as boiler water or combustion air preheating, is considered. Steam used by the boiler water deaerator is estimated at 2% of the total steam consumption (Reid & Rein, 1983). A provision is made for steam losses following recommendations by Rein (2007). The cooling tower is modelled by a flash unit operating at the cooling water temperature and the corresponding vapour pressure of water. In principle, due to evaporation losses in the cooling tower, using some make-up water might be necessary. However, due to the water contained in raw cane, the sugar mill generates large amounts of water effluent (condensed vapours). In the model the effluent is discharged at two points: firstly, right after the evaporation station, and secondly, just before the cooling tower.

Undetermined sugar losses
Sugar losses due to syrup entrainment and sucrose inversion have been taken into account in modelling the evaporator and pan boiling. The degree of entrainment is specified for the first effect only. For the subsequent effects, the entrainment of syrup droplets is assumed to obey a correlation found by Lionnet (1984), according to which the syrup entrainment flow rate is proportional to the linear velocity of vapour to the power of 1.2 and 1.1 for evaporators and pans, respectively. For the calculation of the sucrose inversion effect, the kinetic model proposed by Vukov (1965) was adopted. Since sucrose conversion is a strong function of temperature, pH and retention time (Schäffler, 1987), the required operating conditions for evaporators and pans were taken from Schäffler (1994) and Anon. (2015), respectively.

Model solution methodology

Degree of freedom analysis
Steady-state mass and energy balances of the individual process units constituting the sugar mill are the central part of the proposed mathematical model. These balances are expressed in terms of process and utility stream variables. In its current version the entire sugar mill model involves 180 process and utility streams. Each stream is described in terms of pressure, temperature, flow rate and composition. As the number of the sugar mill variables is much higher than the number of independent mass and energy balance equations available, a certain number of additional stream and process specifications (diffuser separation coefficients, syrup brix, remelt temperature, C-sugar moisture, degree of sugar inversion, pressures, etc.) must be imposed on the system in order to obtain a unique mathematical solution. The degree of freedom (DOF) index is defined as the difference between the number of independent stream variables and the sum of the number of independent balance equations and the number of additional process specifications. The model is correctly specified, i.e. it can be solved uniquely for stream flow rates or compositions and enthalpies or temperatures, if the plant degree of freedom index is zero.

Model building blocks
Process units of the sugar mill, like those of any other chemical plant, can be classified as mixers, distributors (splitters), separators and reactors. Apart from mixers, these elementary building blocks require some parameterisation. The operation of distributors is described in terms of constant distribution coefficients that apply to the entire input stream. Separators, e.g. evaporators, flash drums and crystallisers, distribute individual input stream components differently. In general, separation coefficients are stream composition and temperature dependent. For sugar mill processes involving a phase change, these coefficients are affected by the thermodynamics of the water-sucrose-impurities system. The vapour-liquid equilibrium (VLE) determines the boiling point elevation (Saska, 2002) and is used to

calculate the amount of water evaporation in evaporators, flash drums and pans. In turn, the solid-liquid equilibrium (SLE) determines the sucrose solubility in impure technical sugar solutions (Vavrinecz, 1962; 1965) and is used to determine the amount of sucrose crystallisation (or dissolution) in pans, crystallisers, centrifuges, the remelter and the dryer. In this case, the phase change is driven by non-equilibrium conditions defined by a specific level of supersaturation in the metastable or intermediate zone. Finally, for reactors, one or more degrees of conversion have to be specified. The complete mathematical description of all the sugar mill building blocks, including material and energy balances, along with specification constraints, is given elsewhere (Starzak, 2016).

Numerical solution strategy

Steady-state mass balances are linear in species flow rates and can be solved easily using elementary methods of linear algebra provided the additional constraints imposed on the plant operation are linear as well. Similarly, energy balances are linear in total flow rates provided temperatures and compositions are known in advance. However, this is rarely the case. There are three basic sources of nonlinearities in the sugar mill model: VLE, SLE and thermophysical properties of steam and sugar solutions. As a result, nonlinear chemical plant models, involving typically several hundred independent process variables, can be solved only by iterative calculation.

Numerous computational methods have been developed in the past to tackle the problem of numerical stability and convergence (Buzzi-Ferraris &Manca, 2006). In general, there are three basic classes of methods: successive substitutions including the Wegstein's variant (weak nonlinearities), Newton-Raphson methods including the Broyden's variant (moderate nonlinearities) and continuation methods (highly nonlinear systems). Although the Newton-Raphson and more advanced methods can significantly improve the numerical stability and rate of convergence, they become extremely memory-expensive and time-consuming for large-scale systems because of the Jacobian calculation. The nonlinearities present in the sugar-mill model are relatively mild, allowing for the application of the method of successive substitutions. In some cases, detaching mass balances from energy balances by pre-assuming and iterating temperatures was necessary. Moreover, the sugar-mill configuration could easily be decomposed, allowing for the natural order of calculation where the calculation starts from the extraction plant, then goes through the clarification, evaporation and crystallisation plants to finally end up with the utilities block. The latter completes the main iteration loop. There are also a number of smaller iteration loops within individual plants that could be executed successively. The evaporation and crystallisation plants are computationally the most intense.

Sugar mill model validation - background

Factory performance indicators

One of the most popular methods of validating nonlinear parametric models is by checking how well the simulated output of the model matches the measured output. Having sufficient reliable measured data is therefore essential for a successful model validation. The measured data used in this study were taken from the 90th Annual Review of the Milling Season in Southern Africa 2014/15 (Smith et al., 2015), where more than 50 different factory performance indicators are reported for all sugar mills operating in the southern Africa region. The data selected for the validation process involved figures collected from seven South African mills that implement both mud filtration and the three-boiling partial remelt scheme in their operations (Umfolozi, Darnall, Gledhow, Noodsberg, UCL Co. Ltd., Eston and Sezela). However, in order to generate a set of data that would represent a generic South

African mill, the original data were averaged across all the seven mills. Table 1 presents a list of the process related factory performance indicators accepted for the model validation procedure. There is also a short list of indicators describing the quality of cane. Both lists consist of four categories of indicators. Group A involves indicators that were measured directly and reported in the annual review of factory figures. Indicators from Group B are also reported figures but have been calculated based on other measured indicators. Group C involves unreported indicators that are generally accepted estimates rather than any systematic measurements. Finally, Group D includes indicators measured in some of the mills but not reported in the annual factory review.

Prediction of pol, refractometer brix and apparent purity

The two most important measurements in sugar mill operations to quantify the content of sucrose and total dry solids in the process streams are pol measured by polarimeter and brix measured by refractometer, respectively. While both are factory figures routinely reported by the SMRI Annual Reviews, the sucrose content *Suc*, hence the true purity *Q*, and the true concentration of dry solids *DS* are generally unavailable. However, from the mathematical modelling view, the situation looks quite opposite. Values of *Q* and *DS* can easily be calculated from the stream compositions predicted by the model, whereas developing physical models of the measured quantities is practically unachievable. In order to overcome this difficulty, a decision was made to use two empirical correlations between the measured and true quantities as originally proposed by Hoekstra (Tongaat-Hulett, unpublished results) and later verified by Love (2002). The first equation uses refractometer brix readings $Brix_{ref}$ to provide estimates of dry solids content *DS*. The second equation correlates pol readings to obtain estimates of the sucrose content Suc (% by weight). The ability of both empirical equations to estimate sucrose and *DS* with reasonable accuracy has been confirmed by Love (2002) for technical sugar solutions of both high and low purity. When combined and solved for the two measurables they give (superscript *MOLC* refers to C-molasses):

$$Pol = \frac{Suc - DS \times H}{1 - H} \tag{1}$$

$$Brix_{ref} = \frac{1 + 0.00066 \times Pol - \sqrt{\Delta}}{2 \times 0.00066} \tag{2}$$

where

$$\Delta = (1 + 0.00066 \times Pol)^2 - 4 \times 0.00066 \times DS \tag{3}$$

$$H = \frac{Suc^{MOLC} - Pol^{MOLC}}{DS^{MOLC} - Pol^{MOLC}} \tag{4}$$

$$DS^{MOLC} = Brix_{ref}^{MOLC} \left[1 - 0.00066 (Brix_{ref}^{MOLC} - Pol^{MOLC}) \right] \tag{5}$$

Hoekstra's correlations are not based on any comprehensive data analysis involving streams of a broad range of grades but rely on an *ad hoc* assumption that the factor *H* stays constant for many impure sucrose streams. According to Equations (4) and (5), the evaluation of this factor requires measured values of sucrose content, pol, and refractometer brix. Currently, routine sucrose analyses are performed for mixed juice and C-molasses only. Hoekstra evaluated the *H* factor using data for C-molasses encountered in the South African sugar industry and the same approach was used in this study. Consequently, data used in these correlations must always be expressed on an insoluble solid-free basis.

Table 1. Factory performance indicators considered for the model validation procedure.

Sugar extraction	01 [B]	C-massecuite apparent purity (pan)	33 [A]
Bagasse pol	02 [A]	C-massecuite % crystal content (pan)	34 [B]
Bagasse % moisture	03 [A]	C-molasses @ 85 brix % on cane	35 [A]
Bagasse % fibre	04 [B]	C-molasses refractometer brix	36 [A]
Imbibition % on fibre	05 [A]	C-molasses apparent purity	37 [A]
Extraction pol factor	06 [B]	Remelt apparent purity	38 [A]
Extraction brix factor	07 [B]	A molasses-massecuite ML true purity diff. (cryst.)	39 [C]
Draft juice % on cane	08 [A]	B molasses-massecuite ML true purity diff. (cryst.)	40 [C]
Draft juice refractometer brix	09 [A]	C molasses-massecuite ML true purity diff. (cryst.)	41 [C]
Draft juice apparent purity	10 [A]	A-pan massecuite temperature, °C	42 [C]
Draft juice true purity	11 [A]	B-pan massecuite temperature, °C	43 [C]
Draft juice suspended solids, % DJ	12 [A]	C-pan massecuite temperature, °C	44 [C]
Limestone, t/1000 t dry A-sugar	13 [A]	A-crystalliser massecuite temperature, °C	45 [C]
Clear juice refractometer brix	14 [A]	B-crystalliser massecuite temperature, °C	46 [C]
Clear juice apparent purity	15 [A]	C-crystalliser massecuite temperature, °C	47 [C]
Filtrate apparent purity	16 [A]	A-exhaustion index	48 [B]
Filter cake % on cane	17 [A]	B-exhaustion index	49 [B]
Filter cake pol	18 [A]	C-exhaustion index	50 [B]
Filter cake % moisture	19 [A]	Dry A-sugar pol	51 [A]
Filter wash index	20 [B]	Dry A-sugar % moisture	52 [A]
Syrup refractometer brix	21 [A]	Boiling house recovery	53 [B]
Syrup apparent purity	22 [A]	Undetermined sugar losses, % sugar in cane	54 [B]
A-massecuite (pan), m^3/t DJ brix	23 [A]	Cane-to-sugar ratio	55 [B]
A-massecuite refractometer brix (pan)	24 [A]	Steam-to-cane ratio	56 [D]
A-massecuite apparent purity (pan)	25 [A]		
A-molasses apparent purity	26 [A]		
B-massecuite (pan), m^3/t DJ brix	27 [A]	Cane flowrate, t/h	*01* [A]
B-massecuite refractometer brix (pan)	28 [A]	Cane % sucrose	*02* [A]
B-massecuite apparent purity (pan)	29 [A]	Cane pol	*03* [A]
B-molasses apparent purity	30 [A]	Cane refractometer brix	*04* [A]
C-massecuite (pan), m^3/t DJ brix	31 [A]	Cane apparent purity (DAC)	*05* [A]
C-massecuite refractometer brix (pan)	32 [A]	Cane % fibre	*06* [A]

Model performance index

The task of the sugar mill model validation was formulated as a classical nonlinear least-squares problem. The validity of model predictions was checked against factory data obtained from several sugar mills operating in South Africa. The data included a large number of process indicators characterising the performance of various units constituting the sugar mill. The data structure and their relation to the process variables were discussed in detail in a previous section. The following model performance index was introduced as the most suitable metric to assess the quality of the data fit:

$$I(\mathbf{x}) = \sum_i \frac{w_i \left[FI_i^{pred}(\mathbf{x}) - \overline{FI}_i^{exptl} \right]^2}{\mathrm{var}(\overline{FI}_i^{exptl})} \tag{6}$$

where FI_i^{pred} and $\overline{FI}_i^{exptl}$ are predicted and mean measured values of the i-th factory process indicator, $\mathrm{var}(\overline{FI}_i^{exptl})$ is the variance in the measured values of the i-th factory process indicator, $\mathbf{x}$ is the vector of data regression variables and w_i is an additional weighting factor. As the factory data involved values from seven selected sugar mills, the mean value and the variance represent the implemented data averaging procedure. The inclusion of variances as normalisation factors results in those indicators that show a large scatter of values for different mills having a much smaller impact on the performance index than those which exhibit a good consistency. For example, all factory data on refractometer brix of C-massecuite lie in a very narrow range of values, [92.55, 93.00, 92.51, 92.38, 92.35, 92.90, 92.79], resulting in a small variance of 0.0676. Contrarily, factory data for the filter cake % on cane show a significant scatter across the mills, [2.34, 7.72, 3.36, 6.00, 1.03, 1.10, 1.20], producing a huge variance of 7.02. As a result, the first indicator contributes towards the value of $I(\mathbf{x})$ more significantly. Such a formulation of the performance index allows for prioritising factory indicators in some rational way according to their importance and/or reliability. The additional weighting factor w_i ($0 \le w_i \le 1$) was introduced to allow for data discrimination in dubious cases. By default, for A- and C-category indicators, $w_i = 1$ was assumed while for B- and D-category, $w_i = 0$ (non-optimised).

Data regression variables

Although for a given simulation all sugar mill inputs and other specifications are fixed variables or parameters, their actual values are subject to some uncertainty. In light of the model validation task, they can potentially be treated as model regression variables, which can be used within a certain range of values to minimise the model performance index. However, this should be done with care since some process specifications are strictly controlled in the mill and their variability may be very limited. The complete list of 194 variables that were considered during the validation process is available elsewhere (Starzak, 2016). The decision on which of these were finally used as optimising variables and which were fixed up front was arbitrary, but based on rational arguments.

Solubility coefficient equation

Preliminary calculations showed clearly that the boiling house operations constitute the crucial part of the sugar mill model and simulation results of the crystallisation plant depend heavily on the type of equation used for the solubility coefficient SC, often incorrectly referred to as the saturation coefficient. In general, the equation describes a relationship between SC and the non-sucrose-to-water ratio (NS/W). Occasionally, other effects such as temperature or the ratio of reducing sugars (RS) or monosaccharides (MS) to ash are also accounted for. The relationship has been established relatively well for impure beet sugar solutions (Vavrinecz, 1978/79) but poorly for cane-derived media. Several investigators have studied sucrose solubility for low-grade cane massecuites but there is significant variation between the published results. Figure 2A shows correlations developed by different authors. Clearly, for low-purity streams, the predicted sucrose solubilities differ by as much as 40%. The reason for these large discrepancies is the variable chemical nature of impurities, especially the proportion between organic and inorganic constituents. Monosaccharides generally have a negative effect on the solubility, i.e. sucrose solubility in solution is lower than that in pure water. In contrast, as shown in Figure 2B, monovalent cations such as K^+ and Na^+ have a strongly positive effect. At the origin of the problem is the non-sugar composition of cane, which depends on climatic and soil conditions prevailing in different geographic zones but also in different seasons.

The following mathematical formula is recommended for the relationship between the solubility coefficient and the non-sucrose/water ratio (van der Poel, 1998; Rein, 2007):

$$SC = a\frac{NS}{W} + b + (1-b)\exp\left(-c\frac{NS}{W}\right) \tag{7}$$

The formula does not differentiate impurities and treats them as an additional third component of the solution (*NS*). For the reasons mentioned earlier, parameters *a*, *b* and *c* in Equation (7) are highly specific and values reported by various authors differ substantially (Rein, 2007). In order to overcome this problem, it was decided to estimate these coefficients along with other parameters of the sugar mill model. Furthermore, the effect of temperature seems to be controversial. Some authors neglect it as practically negligible. However, Rouillard (1980) demonstrated for low-grade streams that SC decreases by 10-15% between 30 and 60ºC. Following suggestions made by some authors (Rouillard, 1980; Steindl et al., 2001), a linear temperature dependence of the *b* parameter was assumed (*t* in ºC):

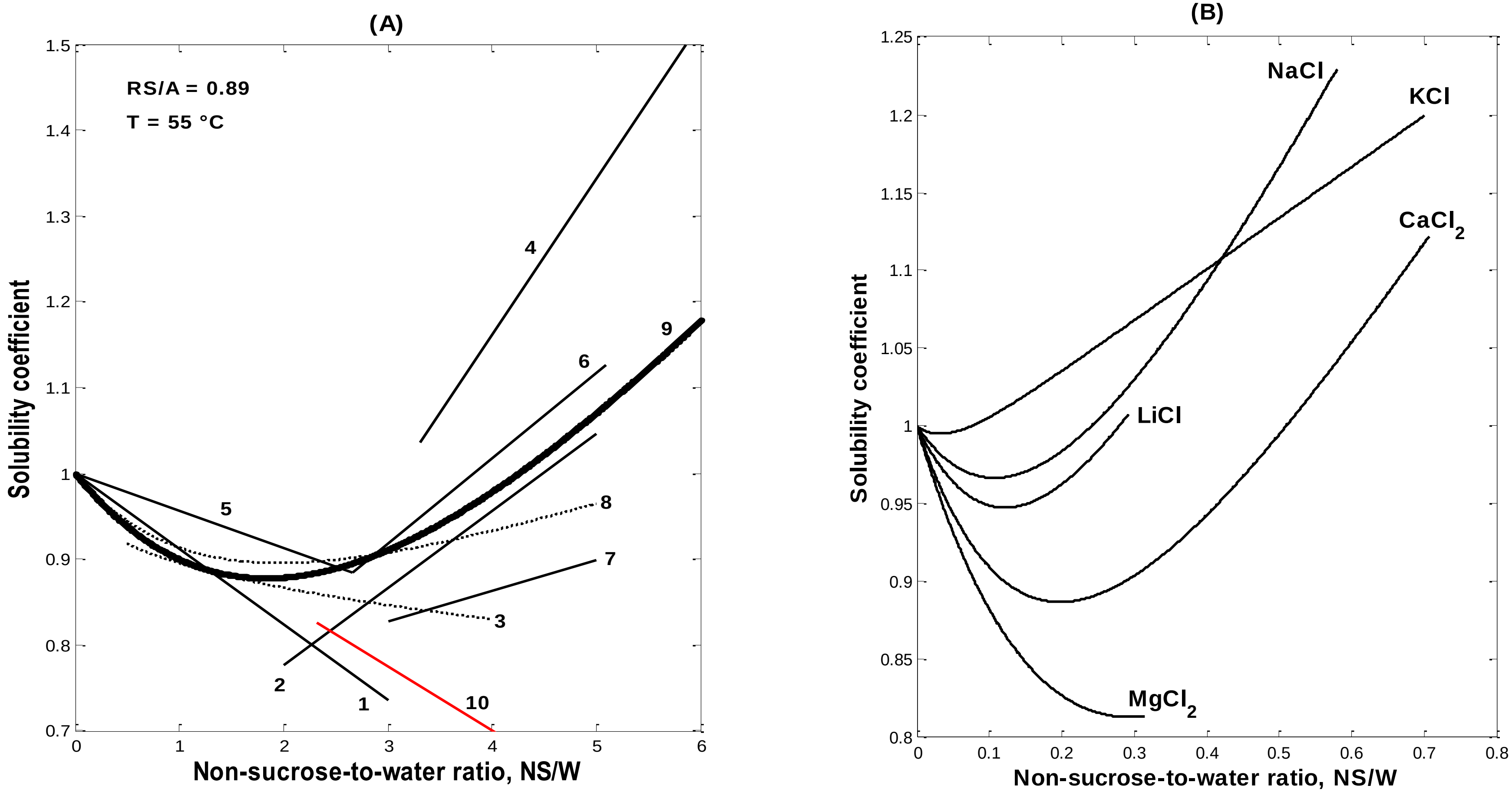
$$b(t) = b_0 - b_1 t \tag{8}$$

A typical *SC* curve exhibits a characteristic behaviour with a minimum value located in the region of reduced solubility. For high-purity mother liquors (NS/W<2), the overall effect of impurities is expected to be negative and the exponential term dominates over the linear term. In turn, for low-purity streams, the exponential term becomes negligible and the curve shows a straight-line behaviour with a positive effect on the solubility. This observation prompted Jesic (1977) to consider a three-parameter broken-line model represented by two straight lines having opposite slopes:

$$SC_{LOW} = 1 - c\frac{NS}{W}, \qquad \frac{NS}{W} \le \frac{1-b}{a+c} \tag{9}$$

$$SC_{HIGH} = a\frac{NS}{W} + b, \qquad \frac{NS}{W} > \frac{1-b}{a+c} \tag{10}$$

The broken-line model has been investigated in this study as the simplest attempt at the complex problem of solubility coefficient modelling.



1 - Batterham et al. (1974)
2 - Maudarbocus& White (1978)
3 - Broadfoot & Steindl (1980)
4 - Lionnet & Rein (1980)
5, 6 - Rouillard (1980)
7 - Broadfoot (1984)
8 - Steindl et al. (2001)
9 - Rein (2007)
10 - Jesic (1977)

Figure 2. Solubility coefficient: (A) effect of the non-sucrose/water ratio; (B) effect of single electrolytes (Quentin, 1960).

Results of sugar mill model validation

Out of 194 variables that had to be specified to run sugar mill simulations, 93 were optimised to get the best data fit in terms of the model performance index as defined by Equation (6). Other variables were fixed by assigning to them some generally accepted values. In order to ensure the stability and fast numerical convergence of calculations, the constrained Nelder-Mead method of optimisation, also referred to as the simplex method, was used. This method is particularly suitable for highly multi-dimensional problems. A reasonable estimate of model parameters could be achieved after 4000-6000 evaluations of the performance index, equivalent to the same number of complete sugar mill simulations. As the solubility coefficient appeared to be the critical element of the crystallisation plant modelling, model validation calculations were performed in two phases.

Factory data regression - Phase I

The following three different SC models were evaluated in this preliminary phase of calculations:

- broken-line model, Equations (9-10);
- exponential model, Equation (7);
- exponential model with temperature dependence, Equations (7-8)

After a few thousand iterations, the nonlinear data regression of the broken-line model resulted in a satisfactory fit of all factory performance indicators, except one - A-massecuite refractometer brix - in which case the error exceeded one standard deviation by nearly 50% (Figure 3). Nevertheless, predicted values of the solubility coefficient quite closely followed the experimental straight line relationship reported by Lionnet and Rein (1980) for low-grade massecuites ($3<NS/W<5$) as shown in Figure 4. It was then found that the continuation of computations resulted in a significant improvement of the data fit, but at the expense of the solubility coefficient broken-line behaviour, which moved away from the Lionnet-Rein experimental line by 5-10%. In both cases the broken-line SC exhibited a minimum in the region of the negative solubility effect for higher grade streams. The regressed parameters of the broken-line model were used to work out first guesses for the exponential model. The behaviour of the two models turned out to be quite similar. This was not surprising as the broken-line model is the simplest possible non-smooth approximation of the exponential model with all basic features retained. The only appreciable difference was a more pronounced SC minimum and a slightly enlarged region of the negative solubility effect. The addition of the temperature effect to the solubility model produced very little improvement. Although a good factory data fit was achieved, the predicted solubility coefficients were still 2-4% above the Lionnet-Rein correlation.

Factory data regression - Phase II

Regression results of the three investigated models of the solubility coefficient showed clearly that keeping all the errors within the standard deviation margin and simultaneously matching the Lionnet-Rein line was technically unfeasible with the model performance index used thus far. It was decided therefore to modify the model performance index by adding to it one more factory performance indicator which would guarantee close proximity to the Lionnet-Rein line. A value of the solubility coefficient taken from the centre of this line (at $NS/W = 5.3$) was chosen as an auxiliary factory data point. This forced the searching algorithm to stay near to the anticipated values of the solubility coefficient and ultimately proved successful. The key results of this calculation are shown in Figures 5 and 6. The factory data fit is excellent while the exponential solubility coefficient curve practically

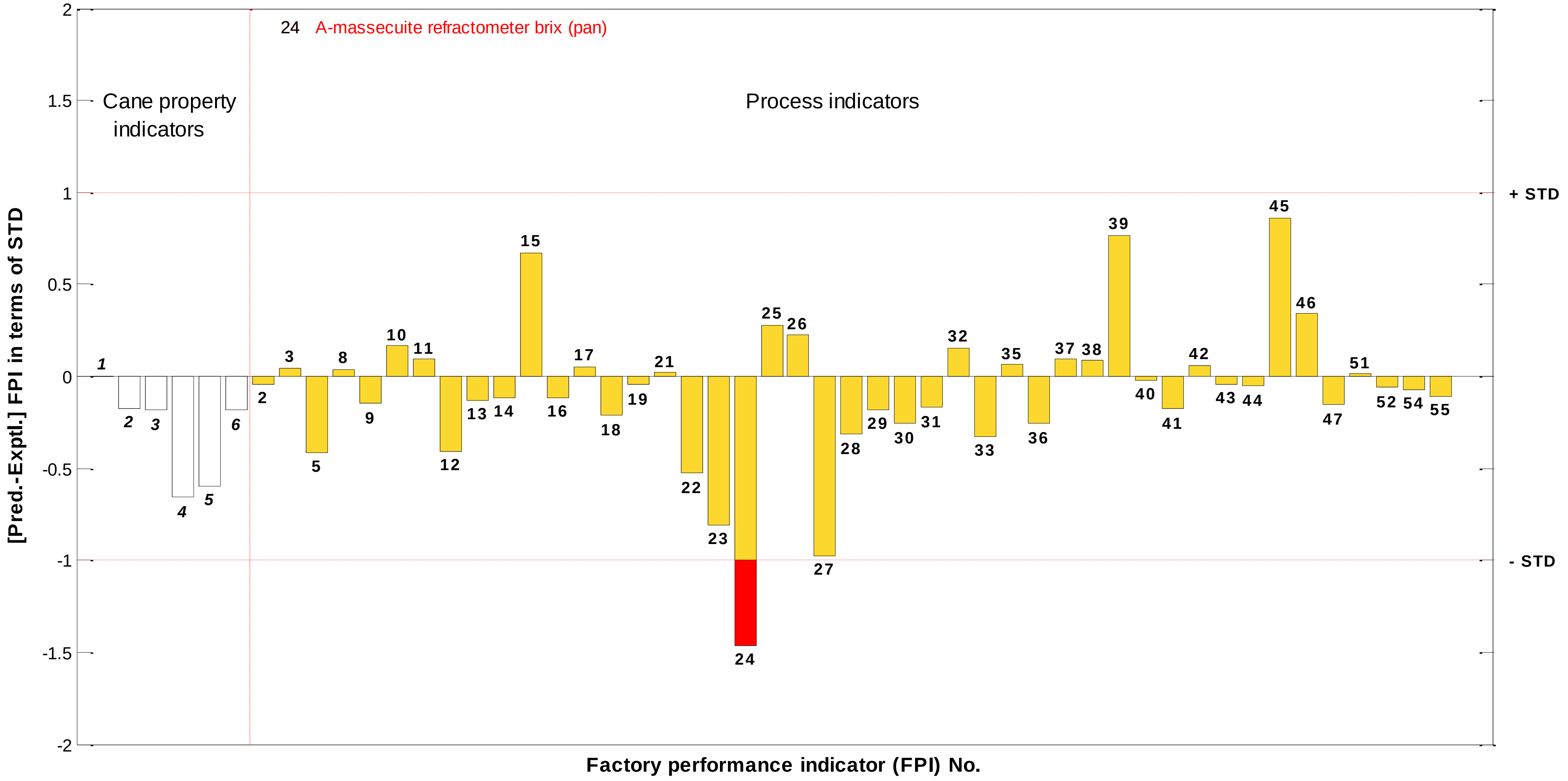


Figure 3. Distribution of optimised Factory Performance Indicators (FPI) for the broken-line model of the solubility coefficient. Indicators are numbered according to the list presented in Table 1.

coincides with the Lionnet-Rein line in its straight line segment valid for low-purity sugar streams. In addition, the region of the negative solubility effect seems to be sufficiently large, extending to NS/W of about 2. The sugar mill model can predict non-optimised factory performance indicators as well. As shown in Figure 7, the data fit here is also quite satisfactory with practically only one indicator, extraction pol factor, clearly exceeding the acceptable margin of error, most likely due to large uncertainty in predicting cane pol from Equation (1)). Numerical values of selected factory performance indicators of the boiling house are presented in Table 2. A complete set of numerical data generated by the computer program for the model validated in Phase II, including the list of estimated and fixed parameters, optimised sugar mill performance indicators and simulated stream data, can be found elsewhere (Starzak, 2016).

When commenting on the final result of data regression it is important to emphasise the fact that out of all experimental solubility coefficient relationships presented in Figure 2A, the Lionnet-Rein correlation yields considerably higher values. However, since the study was done on South African massecuites from the KwaZulu-Natal region, we consider this correlation with greater confidence than those developed using data from Australian or Hawaiian mills. Elevated values of the saturation coefficient would indicate a significant percentage of potassium ions in the inorganic component of cane impurities which can possibly be explained as a result of intensive K-fertilisation of sugarcane.

Supersaturation

The overwhelming majority of the optimised process variables are within the expected range of values. However, one particular parameter characterising boiling house operations can be subject to debate. This is the supersaturation of mother liquor. The predicted mother liquor supersaturation of massecuite out of the A-pan is 1.336, practically very close to the critical boundary of the metastable zone. Supersaturation values for B and C pans show a decreasing trend (1.211 and 1.130, respectively) whereas one would expect slightly higher values and not very different from each other. No particular pattern is observed for supersaturations in massecuite streams leaving the crystallisers (1.349, 1.050 and 1.088 for A, B and C crystallisers, respectively). Nevertheless, for the A crystalliser one would expect a considerably lower value indicating more profound exhaustion of the crystallisation driving force. On the other hand, significant temperature changes of 15-20ºC between pans and crystallisers create a situation in which the level of supersaturation can be maintained, giving rise to the desired high crystallisation rates.

Certainly, more realistic modelling of the crystallisation phenomenon in both pans and crystallisers could shed more light on the controversial supersaturation figures. For example, the model currently used for the A pan ignores the fact that this is a two-stage operation and a batch, rather than perfectly-mixed, flow process should be considered. In turn, the continuous operating regime of crystallisers, close to a tanks-in-series arrangement, makes it more similar to a plug-flow apparatus than a well-mixed vessel. It is difficult to say firmly that this would be a remedy to the problem because actual values of supersaturation are not known and hence proper comparison cannot be made. Interestingly, most of the authors who advise the critical limit data for the metastable zone do not pay any attention to the lack of reliable instruments capable to fill the need for on-line data capture (Rózsa, 2008). Various authors report different figures ranging from 1.12 to as much as 1.46 for pan massecuites (Graham, 1966) and from 1.19 to 1.41 for crystalliser massecuites, depending on the cooling regime applied (Hedley, 1937). In addition, the uncertainty is deepened by the fact that supersaturations depend on running temperatures that are variable and known only approximately as “expected values”.

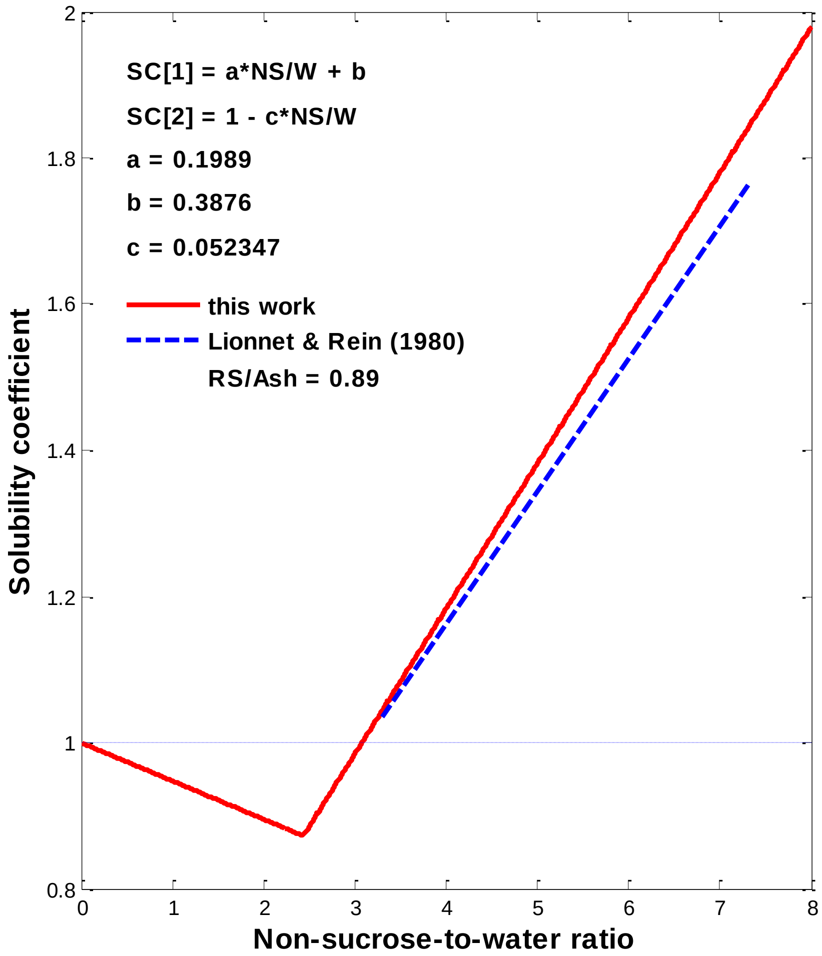


Figure 4. Solubility coefficient vs non-sucrose-to-water ratio (NS/W) for the broken-line model.

Steam consumption

According to Rein (2007), the lower limit for steam consumption using present technology and extensive process integration is estimated at 0.33-0.35 t per tonne of crushed cane. However, the reality for most of the sugar mills is that this value lies somewhere between 0.4 and 0.6 t/t cane. The boiler steam consumption predicted by the model was found to be 0.396 t/t cane. As no reliable systematically recorded data on steam consumption in the local sugar mills exist, this figure could not be properly validated. There is, however, a general opinion based on some rough estimates that South African sugar mills are energy inefficient and the steam consumption is significantly higher than in other parts of the world. Reid & Rein (1983) performed a detailed analysis of the Felixton II mill and estimated the steam requirement at 0.48 t/t cane. Certainly, the figure produced by the model is underestimated. Firstly, no provision was made for steam used for sundry heating throughout the factory, which is typically estimated at 6% (Reid & Rein, 1983) or higher (Rein, 2007) and, secondly, increasing the steam demand by the deaerator to 8-9%, as reported by Rein (2007), would also bring the predicted total steam consumption closer to the realistic level.

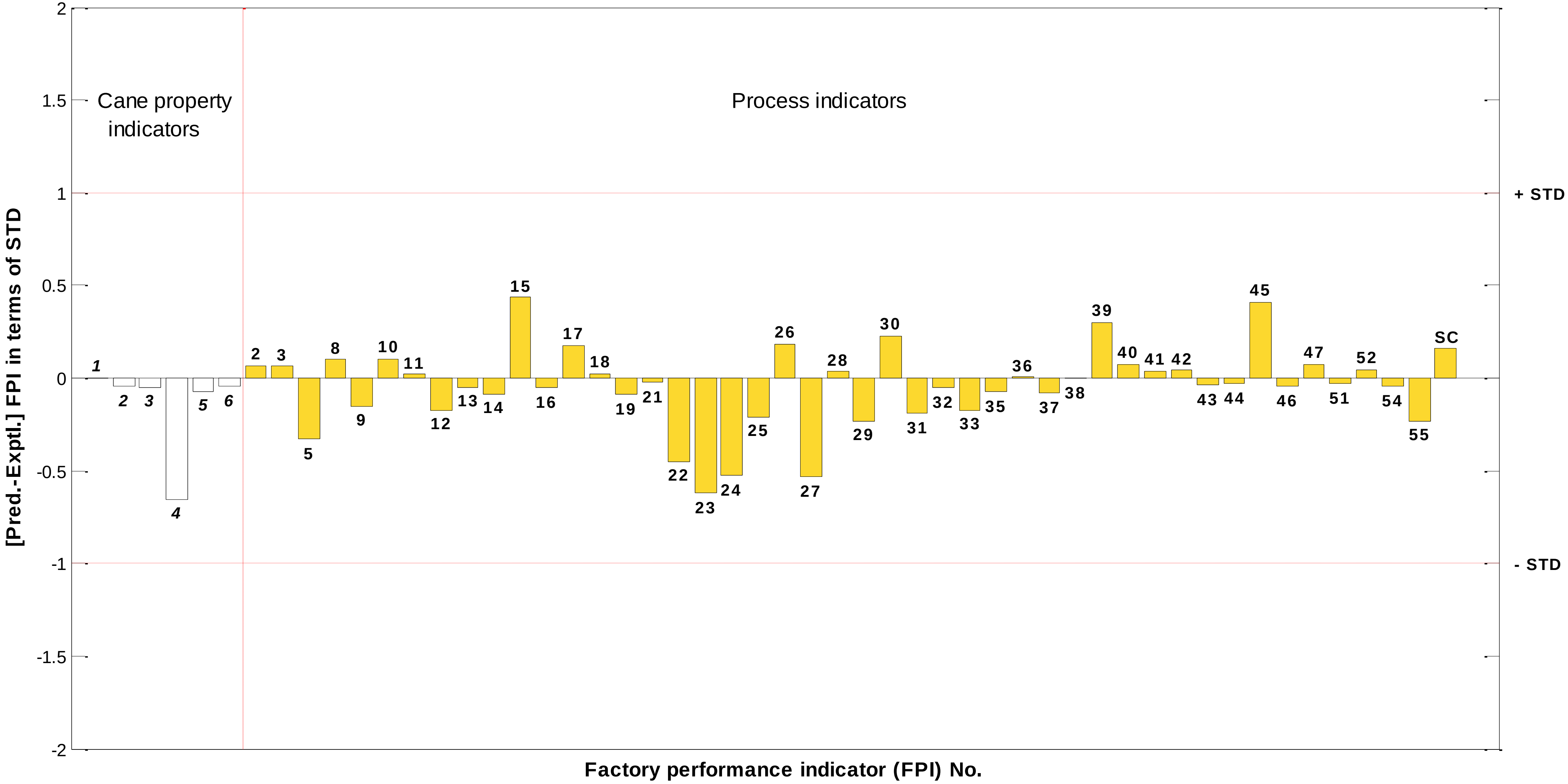


Figure 5. Distribution of optimised factory performance indicators for the exponential model of the solubility coefficient. Indicators are numbered according to the list presented in Table 1.

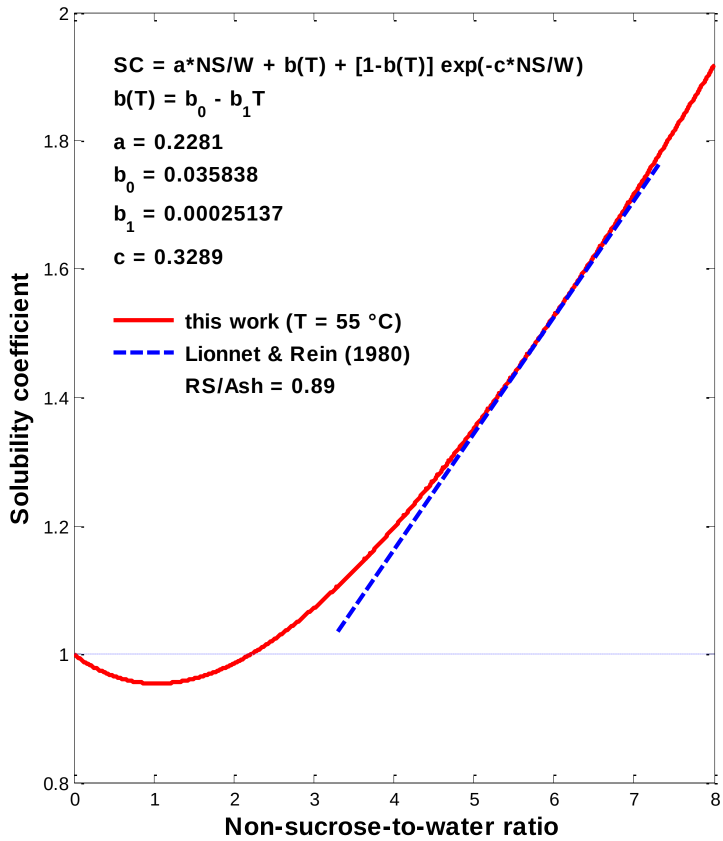


Figure 6. Solubility coefficient vs non-sucrose-to-water ratio (NS/W) for the exponential model.

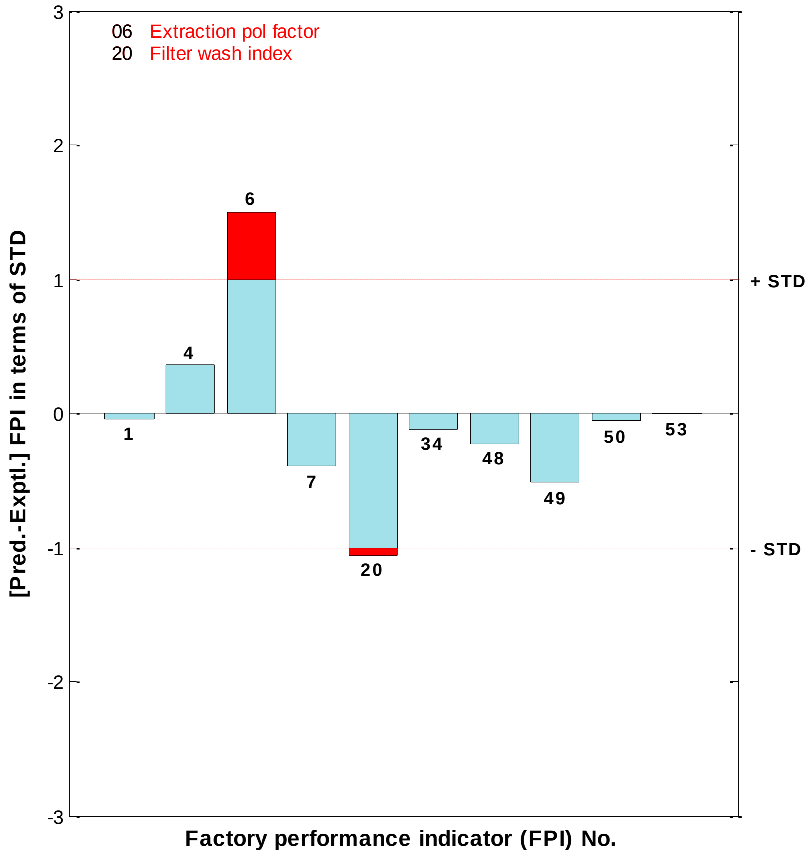


Figure 7. Distribution of non-optimised factory performance indicators for the exponential model of the solubility coefficient. Indicators are numbered according to the list presented in Table 1.

Table 2. Selected factory performance indicators of the boiling house.

Optimised FPI	Actual	STD	Predicted	Deviation
Massecuite, m^3/t DJ brix				
A	1.05	±0.09	0.99	-0.06
B	0.40	±0.05	0.37	-0.03
C	0.27	±0.03	0.26	-0.01
Massecuite, ref. brix, %				
A	92.64	±0.26	92.51	-0.14
B	94.64	±0.46	94.66	+0.01
C	96.96	±0.61	96.93	-0.03
Massecuite, app. purity, %				
A	85.68	±0.72	85.60	-0.08
B	69.74	±1.16	69.58	-0.16
C	54.20	±1.33	53.97	-0.23
Molasses, ref. brix, %				
C	81.92	±1.98	81.93	+0.01
Molasses, app. purity, %				
A	69.55	±1.89	70.00	+0.45
B	47.24	±1.44	47.65	+0.41
C	35.86	±1.33	35.76	-0.10
Remelt, app. purity, %	85.49	±0.64	85.49	0.00

Non-optimised FPI	Actual	STD	Predicted	Deviation
Boiling house recovery, %	85.65	±1.90	85.74	+0.09
A exhaustion index, %	61.66	±4.01	60.77	-0.89
B exhaustion index, %	61.14	±1.95	60.21	-0.93
C exhaustion index, %	52.70	±3.03	52.52	-0.18

Conclusion

A sugar-mill model was developed with the intention to create a firm mathematical representation of a generic South African mill. The model has been validated using averaged factory data from seven sugar mills located in KwaZulu-Natal. The validation process, which fits 51 factory performance indicators, involved the optimisation of 93 sugar mill operating variables and parameters. The correlation describing the solubility coefficient appeared to play the critical role in the prediction of the boiling house performance. A solubility coefficient equation, specific to sugar streams encountered in the South African sugar industry and in-line with the earlier work of Lionnet and Rein (1980), was developed and resulted in the successful regression of all measured factory performance indicators within a standard deviation error margin.

The validated MATLAB® model of the sugar mill is currently being transferred to an Aspen Plus®-based platform to permit extension to new biorefinery products that, in general, cannot be easily handled in MATLAB® due to the lack of a comprehensive physical property database. The AspenPlus® model will serve as a starting point on which future downstream processes can be attached.

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