

# PROGRAM FOR SIMULATING AND EVALUATING A CONTINUOUS A-SUGAR PAN

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## Abstract

The Continuously Operating Raw Pan Simulation and Evaluation (CORPSE) is a steady-state computerised simulation of such a pan, based on the solution by the Newton-Raphson method of simultaneous algebraic equations which describe the mass and heat transfer within and the material balances over each compartment. Each compartment is considered as a stirred tank reactor, with unknown components being: Total solids, total sucrose, crystal sucrose and water. Other unknowns could include compartment volumes and process values such as pan vapour pressure, supersaturation and mass and heat transfer coefficients. The user of the model has considerable freedom of choice of input data.

This model has been used for:

- Evaluating process parameters from observations of an operating pan. If more than the minimum amount of data is submitted, the program performs a least-squares fit.
- Sizing of compartments and calandria heat transfer areas for design purposes.
- Showing how different values of controllable process variables affect the operation of the pan.

## 1. Object

The computer program for the Continuously Operating Raw Pan Simulation and Evaluation (CORPSE) was developed with the following objectives in mind:

- (a) Evaluation Mode:  
To determine the main process parameters of an existing pan from measurements taken during factory operation.
- (b) Design Mode:  
To size the volumes and heat transfer areas of future pans, using the above obtained parameters together with the operating specifications.
- (c) Operation Mode:  
To show the quality and quantity of product which will be produced from the interaction of a given set of controllable operating variables.

## 2. Approach

- (1) CORPSE is to be a steady-state simulation. This requirement is obvious from objectives (a) and (b) above, and the object of (c) was also to show steady-state operation rather than to demonstrate dynamic response to changes in controllable process variables.
- (2) The number of compartments can be varied, to make CORPSE applicable to various installations.
- (3) Many simplifying assumptions have to be made: sometimes for lack of accurately known relationships; sometimes in order to keep the mathematics manageable. Because the same simplifying assumptions are used in all three modes, it is reasonable to expect that, by applying the same values of parameters obtained in the Evaluation mode to the Design and Operation modes, the results obtained in the simulations will be sufficiently in accord with practice.

- (4) Each of the compartments is to be considered as a stirred tank reactor. For the continuous pans on which Rein *et al*<sup>13</sup> have performed lithium tracer tests, it was found that one compartment could effectively represent anything from 1 to 2 equivalent stirred tanks. Such evidence was not sufficiently conclusive to justify the complicated modelling necessary for assuming anything other than one stirred tank per compartment.
- (5) The number of crystals is assumed to remain constant from entry to exit of the pan. When operating an A-pan, the crystals in the seed stream will have already grown to a fair size in a batch pan. If excessive under- and supersaturation respectively are avoided, there should be neither disappearance of crystals through dissolution nor creation of new crystals through spontaneous nucleation.
- (6) Within each compartment, the processes of heat transfer from the calandria into the massecuite and of mass transfer of dissolved sucrose from the mother liquor onto the growing crystals are simulated. Mass balances across that compartment are also taken.
- (7) The simulation could be based on one of the following methods:
  - (a) Simulation of each compartment in turn:  
The first compartment is simulated by using the values of the input streams, thus calculating the values of the output streams, and from there on to the second compartment, etc. However, some of the necessary data for the simulation will usually be unknown, such as parameters (when in Evaluation mode) or compartment volumes and areas (when in Design mode). This would require using initial estimates of the unknowns and repeating the calculating cycle over the successive compartments several times.
  - (b) Simultaneous simulation of all compartments:  
This is performed by setting up the appropriate equations for each of the compartments, and solving them all as a set of simultaneous algebraic equations. Because not all the equations are linear, they have to be solved by an iterative mathematical method, with initial estimates of the unknowns.

It was decided to use the method (b) of simultaneous equations, using the Newton-Raphson method of solution.

Although it requires more computer capacity, it is a more orderly method and allows greater flexibility of choice of which shall be the given input values and which the unknown values to be determined by CORPSE. For each given value in the input data, CORPSE sets up an appropriate equation. Furthermore, when in the Evaluation mode, it is possible (and indeed desirable) to over-specify the system with whatever plant observations are available, meaning that there will be more relationships (equations) than unknowns.

In such a case, the Newton-Raphson method can be adapted to perform a least-squares fit to determine the most likely values of unknowns from all the data.

## 3. Schematic representation of a Continuous Pan

This is shown in Figure 1 for a pan of N compartments, numbered 1 to N.

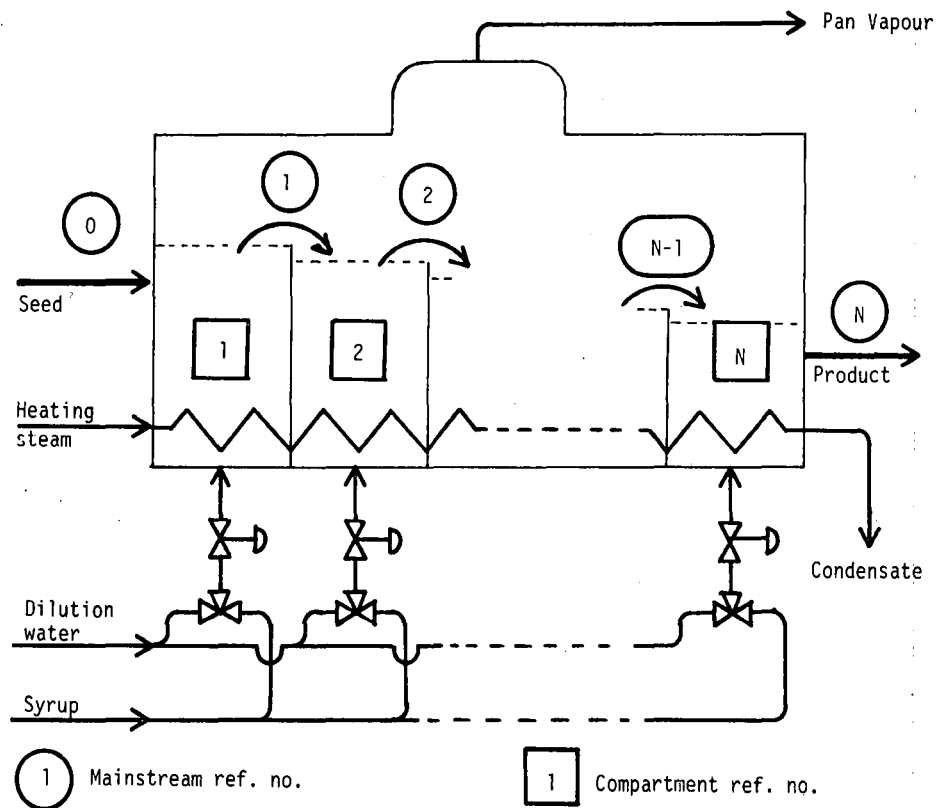


FIGURE 1 Diagrammatic representation of a continuous pan.

The compartments are connected in series, and share a common pan vapour space and a common calandria steam supply.

The mainstream enters compartment 1 as the seed stream. The contents of compartment 1 overflow via a weir into compartment 2, and so on. The mainstream leaving compartment N is the product stream.

Because of the assumption that each compartment, say No. J, is a perfectly stirred tank, it follows that its contents will have the same composition as the mainstream leaving it, which should logically be called mainstream No. J. For convenience the seed stream is referred to as mainstream No. 0.

The composition and mass rate of the mainstream are completely specified by the following components, with dimension tons/h:

- water
- crystal sucrose
- total sucrose, which consists of dissolved as well as crystal sucrose
- total solids, which consists of total sucrose plus non-sucrose. The non-sucrose is all in dissolved form.

Each of the N compartments has 2 auxiliary feeds to it, syrup and dilution water. These feeds share a common control valve per compartment, and either the one or the other is fed to the compartment. The syrup feed has the components water, total sucrose and total solids, but no crystal sucrose.

#### 4. The Unknowns

There are many variables in a continuous pan. Initially the values of most are unknown, and have to be calculated by running the mathematical model. All these unknowns can however be reduced to a set of primary unknowns, which are tabulated as follows:

TABLE 1  
Primary unknowns

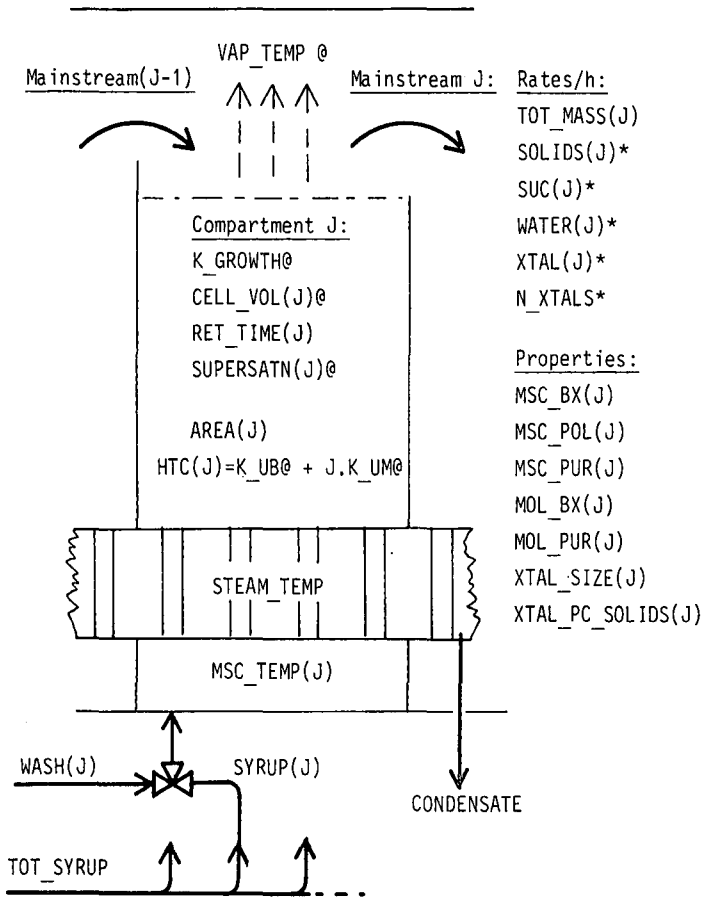
Symbolic Representation	Description	Dimensions	Indexing	
<b>The following will always be unknowns:</b>				
SOLIDS(J)	Mass rate of total solids in mainstream	tons/h	J= 0 to N	
SUC(J)	Mass rate of total sucrose in mainstream	tons/h	J= 0 to N	
WATER(J)	Mass rate of water in mainstream	tons/h	J= 0 to N	
XTAL(J)	Mass rate of crystal sucrose in mainstream	tons/h	J= 0 to N	
N_XTALS	No. of crystals in mainstream	$\times 10^9/h$	None	
<b>The following can be additional unknowns for the Evaluation Mode:</b>				
K_GROWTH	Crystal growth rate parameter Parameters of linear function of heat transfer coeff. w.r.t. compartment no.	mm/h	None	
K_UB		Intercept	$kw/(m^2C)$	None
K_UM		Slope	$kw/(m^2C)$	None
K_SUPERSATN	Common value of supersaturation	—	None	
<b>The following can be additional unknowns for the Design Mode:</b>				
CELL_VOL(J)	Effective volume per compartment	$m^3$	J= 1 to N	
STEAM_TEMP	Temp. of heating vapour to calandria	$^{\circ}C$	None	

CORPSE sets up the equations in terms of these primary unknowns and solves for them. From this solution, all the other unknown values can be calculated.

An illustration of the variables w.r.t. one compartment, say compartment J, is shown in Fig. 2.

#### 5. Data which can be available as input to CORPSE

The user has considerable choice of what data to input to the model. This will depend on the purpose he wants to use



\* = Will always be a primary unknown  
 @ = Can be a primary unknown

FIGURE 2 Variables w.r.t. compartment J of a continuous pan.

CORPSE for as well as what data are available. The amount of data must of course be sufficient so that the number of equations which CORPSE will set up will be at least equal to the number of unknowns. That in itself is no absolute guarantee that the equations can be solved, because the user must still beware of the possibility that the system is overspecified in one part and underspecified in another. The following list gives the possible data which can be specified as input:

**Performance Data:**

- Feed rate of seed stream.
- Output rate of massecuite stream.
- Total feed rate of syrup.
- Total production rate of calandria condensate.

Solids % Total mass }  
 Sucrose % Solids } of massecuite, for mainstreams 0  
 Crystal % Solids } to N  
 Purity }  
 Crystal sizes }

Solids % Total Mass }  
 Sucrose % Solids } of mother liquor (molasses), for  
 Purity } mainstreams 0 to N

Supersaturation of mother liquor } per compartment, for  
 Feed rate of dilution water } compartments 1 to N.

Solids % Total Mass }  
 Purity } of syrup.

Pressure or temperature of calandria vapour.  
 Pressure or temperature of pan vapour.

**Pan construction specifications:**

Volume } per compartment, for compart-  
 Heat transfer area } ments 1 to N.

**Process parameters:**

Crystal growth rate.  
 Heat transfer coefficient per compartment, for compartments 1 to N.

**6. Concept of Mean Crystal Sizes**

As the massecuite moves from compartment to compartment, the linear dimension (length) of each crystal will increase during its stay in that compartment, dependent mainly on the degree of supersaturation and the retention time in that compartment, and on the growth rate parameter for sucrose.

One obviously cannot consider each crystal on its own, so it is therefore necessary to find some general measure of crystal size which is appropriate to the technical context in which it is used in the simulation. This requires a knowledge of the grain size distribution in each of the compartments.

For the purposes of this simulation, 3 different bases of frequency distributions are used:

(a) *Size-frequency-by-number*

This is the fraction  $dn/n$  w.r.t. the total number of crystals  $n$  with sizes (lengths) within the range of  $L$  and  $L + dL$ , where  $n$  = total number of crystals in sample

$L$  = size (length) of crystal

$dL$  = small increment in size  $L$

One would obtain this basis of frequency distribution when examining a representative sample of the massecuite under a microscope with a grid and counting the number of crystals in each size category.

Its application is the following:

Because each individual crystal is subjected to conditions of growth, it is logical when considering growth to define the size of the average crystal as the sum of the sizes of all the crystals divided by the number of crystals, which will be called the *mean-size-by-number*, and is calculated from the size-frequency-by-number distribution.

(b) *Volume-frequency-by-number*

This is the fraction by  $dn/n$  w.r.t. the total number of crystals  $n$  with volumes within the range of  $V$  and  $V + dV$ , where  $V$  = volume of a crystal.

$dV$  = small increment in volume  $V$ .

If the crystals are all of uniform shape, one can have the relationship between volume and length of crystal, namely

$$V = cL^3,$$

where  $c$  = shape factor

= 1 for cubes,

=  $\pi/6$  for spheres, etc.

For CORPSE, the crystals were taken to be cubic, ie  $c = 1$ . One could equally well define the volume-frequency-by-number as the fraction by number  $dn/n$  w.r.t. the total number of crystals  $n$  with volumes within the range of  $cL^3$  and  $c(L + dL)^3$ . Note that this is not the same as the range  $cL^3$  and  $cL^3 + cd(L^3)$ . Its application is when it is required to calculate the total mass of crystals in any compartment, given their total number.

It should be clear that:

Mass of crystals

$$= \text{Mean-volume-by-number} \times \text{Density of crystal} \times \text{No of crystals, where}$$

Mean-volume-by-number can be defined as the sum of the volumes of all the crystals divided by the no. of crystals, and can be calculated if the volume-frequency-by-number distribution is known.

Re-arranging:

Mass of crystals

$$= \frac{\text{Mean-volume-by-number}}{(\text{Mean-size-by-number})^3} \times (\text{Mean size-by-number})^3 \times \text{Density of crystals} \times \text{No. of crystals.}$$

The factor  $\frac{\text{Mean-volume-by-number}}{(\text{Mean-size-by-number})^3}$  will be abbreviated by VL3 and can be calculated for each compartment.

Symbolically, the above expression for crystal mass becomes:

$$\text{XTAL}(J) = \text{VL3} * \text{XTAL\_SIZE}(J) ** 3 * \text{XTAL\_DENSITY} * \text{N\_XTALS}$$

(c) *Size-frequency-by-mass*

This is the fraction by mass dm/m w.r.t. the total mass of crystals m with sizes within the range of L and L + dL, where m = mass of sample.

This basis of frequency distribution is obtained from sieving analyses.

Although it is not directly used in the process relationships of CORPSE, its application is to calculate the *mean-size-by-mass*, or more commonly known as the mean aperture (MA). This measure is often used in the sugar industry and is defined as the sum of (Size × mass per crystal) divided by the total mass of all crystals.

**7. Probability Density Functions:**

*Types*

Various probability density functions (p.d.f.'s) have been considered to describe distribution based on size-frequency-by-number:

- Gamma p.d.f.
- Log-normal p.d.f.
- Rosin-Rammler p.d.f.
- Generalised Negative Exponential p.d.f.

In deciding which of these p.d.f.'s to use, the following must be considered:

- (1) It must be a good fit to the results obtained in practice.
- (2) It should be possible to transform mathematically the p.d.f. on size-frequency-by-number to corresponding p.d.f.'s which describe the volume-frequency-by-number and the size-frequency-by-mass distributions per (b) and (c) above.
- (3) In practice, the size-frequency-by-number distribution is skewed and there obviously cannot be negative size values. This rules out the normal (Gaussian) p.d.f. which is symmetrical and would show a significant proportion of negative sizes at the comparatively high coefficients of variation which crystal size distributions exhibit.

From work which has thus far been done, the generalised negative exponential (GNE) p.d.f. answers fairly well to the above requirements.

*Fitting the p.d.f. in practice*

When performing factory tests it is, for practical reasons, far easier to obtain size-frequencies-by-mass through sieving than size-frequencies-by-number through counting under a microscope. To deal with this, the GNE p.d.f. which describes the size-frequency-by-number was transformed to a p.d.f. which describes the corresponding size-frequency-by-mass, but still

in terms of the same parameters. This last mentioned p.d.f. was fitted to the sieving results by non-linear regression analysis and the values of its parameters determined.

From these parameters the mean-size-by-number, mean-volume-by-number and mean-size-by-mass can be calculated.

Appendix 1 describes the GNE p.d.f., its transformation and the expressions of the above means sizes in terms of its parameters.

*P.d.f. per compartment*

Theoretically, one could start off with a p.d.f. of the crystals in the seed stream and, with consideration of the residence time distributions in each of the theoretical stirred tank reactors, model the size dispersion as well as the increase in mean size of the crystals leaving that compartment. This would however make the mathematics extremely complicated, plus the fact that the changes in size dispersions obtained in practice might in any case not agree with the theoretical.

For those reasons, the following procedure was decided on:

- Take a sample from each of several compartments of an operating pan (in practice, every 2nd compartment).
- On each sample do a sieving analysis and use non-linear regression to calculate the shape parameter of the GNE p.d.f. (See Appendix 1).
- Fit a linear regression relationship between the shape parameter and the compartment no., so that this parameter can be estimated for each compartment. The value of the shape parameter for each compartment gives a measure of the crystal size dispersion, and is used in whatever of the 3 modes (Evaluation, Design, or Operation) it is intended to run the program.

**8. Setting up equations on mainstream properties**

These equations can all be transformed into a pure linear form, and do not pose any problem.

The procedure is to let the stream reference index J go through a DO-loop from 0 to N, examine for which properties are there values given in the input and, if so, set up the appropriate equations. The mainstream properties considered are:

- Crystal size (mm):  

$$\text{XTAL}(J) = 10^9 * \text{N\_XTALS} * \text{XTAL\_DENSITY} * \text{VL3} * ((\text{Given}) \text{SIZE}(J)) ** 3$$

This is a linear equation in the primary unknowns XTAL(J) and N\_XTALS.

- Solids % Total mass in massecuite:  

$$\text{SOLIDS}(J) / (\text{SOLIDS}(J) + \text{WATER}(J)) = (\text{Given}) \text{MSC\_BX}(J) / 100$$

This can be linearised in terms of the primary unknowns:  

$$\text{SOLIDS}(J) - \text{WATER}(J) * \text{MSC\_BX}(J) / (100 - \text{MSC\_BX}(J)) = 0$$

Other properties can similarly be reduced to linear forms:

- Sucrose % Total mass in massecuite
- Purity of massecuite
- Solids % Total mass in molasses
- Sucrose % Total mass in molasses
- Purity of molasses
- Crystal % Total solids
- Mean crystal size. If this is given as mean-size-by-mass (Mean Aperture), it will be converted to mean-size-by-number.
- Total mass flow rate (usually only available for seed or product stream).

### 9. Setting up equations on compartment material balances

These equations can also be linearised, and are set up in a DO-loop over compartments 1 to N.

- Sucrose mass balance:  
 $SUC(J) - SUC(J-1) = (SOLIDS(J) - SOLIDS(J-1)) * (Given) SYRUP\_PUR/100$
- Solids mass balance:  
 $SOLIDS(J) = SOLIDS(J-1) + (Given)SYRUP(J) * (Given) SYRUP\_BX/100$   
 This equation can only be set up for compartments where the amount of syrup feed is known, even if it is zero.

### 10. Setting up equations on processes within compartments

These equations are very much non-linear, and express the fundamental mass and heat transfer processes taking place.

Because they have to be solved simultaneously with all the previously discussed pure linear equations, the Newton-Raphson method is used, whereby the partial derivatives with regard to the primary unknowns form part of the coefficient matrix of the linear equations to be solved. Fortunately these equations, in spite of their complexity, are differentiable, so that the computer program can calculate the values for the expressions of the partial derivatives. In another publication, Hoekstra<sup>6</sup> describes the general principles of the method.

The procedure again is to deal with the compartments in turn through a DO-loop with index J going from 1 to N.

#### (a) Growth rate equation

The basic assumption is that the increase in the linear dimension of a crystal is equal to the growth rate (measured as increase in length per unit time) multiplied by its retention time. According to Wright<sup>14</sup> and Austmeyer<sup>1</sup>, the rate of crystallisation is dependent on crystal size, in that it is proportional to (crystal size)<sup>n</sup>, where Wright estimated  $n = 0,8$ . The relationship proposed by Pot<sup>12</sup> is far more complicated. In view of the seed and product sizes in most applications being of roughly the same respective sizes, and the increase in size usually being by a factor of between 1,5 and 2, it was felt that, for the way in which CORPSE was to be used, the error in letting the growth rate in the model be independent of crystal size would be sufficiently small to justify the gain in simplicity. Gros<sup>5</sup> also ignored the size-dependence effect in his model.

Expressing it in an equation:

$$SIZE(J) = SIZE(J-1) + GROWTH\_RATE * RET\_TIME \dots \dots \dots (1)$$

where  $SIZE(J)$  = Size (length) of crystal, mm

$RET\_TIME$  = Retention time (h)  
 =  $CELL\_VOL(J)/MSC\_VOL$ .

$CELL\_VOL(J)$  = Compartment volume (m<sup>3</sup>). In the Design mode this is one of the primary unknowns, and assumed to be equal for all compartments. A dead-volume fraction of zero is assumed.

$MSC\_VOL$  = Masseccite volume (m<sup>3</sup>/h) which can be empirically expressed in terms of the primary composition variables.

$GROWTH\_RATE$  = Growth rate (mm/h)  
 =  $K\_GROWTH * (SUPERSATN(J) - 1.0046) * TEMP\_EFFECT * EXP(-1.75 * I\_W\_RATIO)$

$K\_GROWTH$  = Growth rate parameter (mm/h). In the Evaluation mode this is one of the process parameters.

$TEMP\_EFFECT$  = Temperature effect on the reaction rate. This is an Arrhenius type function of the masseccite temperature  $MSC\_TEMP$ , per Wright.<sup>14</sup>

$MSC\_TEMP$  = Masseccite temp(°C). This is calculated from the boiling point elevation (BPE) relative to the given pan vapour-temperature  $VAP\_TEMP$ . The BPE(J) is expressed in terms of the primary unknowns in an empirical relationship derived by the author and given in Appendix 2.

$I\_W\_RATIO$  = Impurity-to-water ratio of molasses, which can directly be expressed in terms of the primary unknowns.  
 =  $(SOLIDS(J) - SUC(J))/WATER(J)$   
 The way in which the impurity-to-water ratio affects the rate of mass transfer, as determined by Wright<sup>14</sup> for Queensland syrups, is used.

$SUPERSATN(J)$  = Supersaturation (dimensionless). In the Design and Operation modes this will be given per compartment, and in the Evaluation mode it will be unknown.

For equation (1) the unknown  $SIZE$  must be expressed in terms of primary unknowns:

$$XTAL(J) = 10^9 \times N\_XTALS * XTAL\_DENSITY * VL3 * SIZE(J) ** 3$$

where

$XTAL\_DENSITY$  = crystal density (tons/m<sup>3</sup>)

$VL3$  = factor of mean volume to cubed mean size mentioned in Section 6(b).

In this way it is possible to express equation (1) entirely in terms of the primary unknowns.

#### (b) Supersaturation equation

Whether the supersaturation is itself known or unknown, it has to be expressed in terms of the primary unknowns. The ICUMSA<sup>9</sup> definition of supersaturation can be transformed to:

$$SUPERSATN(J) = SUC\_W\_RATIO * (100 - SOLUB) / (SOLUB * (1 - 0.088 * I\_W\_RATIO)) \dots \dots \dots (2)$$

where

$SUC\_W\_RATIO$  = Sucrose-to-water ratio of mother liquor (molasses)  
 =  $(SUC(J) - XTAL(J))/WATER(J)$

$SOLUB$  = Solubility of sucrose in pure solution (%). This can be expressed in an empirical polynomial equation in terms of  $MSC\_TEMP$ , per Charles<sup>4</sup>.

The effect of the impurity-to-water ratio  $I\_W\_RATIO$  on the solubility of pure sucrose is per Wright<sup>14</sup>.

To obtain meaningful results from plant data when in the Evaluation mode, it is necessary to make the assump-

tion that the unknown supersaturation is the same in all compartments, ie at a common value  $K\_SUPERSATN = SUPERSATN(J)$  for all  $J = 1$  to  $N$ .

(c) *Heat Transfer Equation*

This is another important non-linear relationship in the vacuum pan, which is expressed in terms of some of the process parameters.

Taking a water balance:

- Total water entering compartment J - Total water leaving compartment J
- = Water evaporated
- = Heat transferred through the calandria walls ÷ Latent heat of evaporation.

More specifically, for compartment J:

$$WATER(J-1) + (Given) WASH(J) + SYRUP(J) * (1 - SYRUP\_BX/100) - WATER(J) = 3.6 * HTC(J) * AREA(J) * (STEAM\_TEMP - MSC\_TEMP(J)) / LAT\_HT(VAP\_TEMP) \quad (3)$$

- where WASH(J) = amount of dilution water added (tons/h)
- SYRUP(J) = amount of syrup feed added (tons/h)
- SYRUP\_BX = solids % mass of syrup
- HTC(J) = heat transfer coefficient (kW(m<sup>2</sup>C))
- AREA(J) = heat transfer area of calandria for compartment J (m<sup>2</sup>)
- LAT\_HT(VAP\_TEMP) = latent heat (kJ/kg) of pan vapour, taken to be a linear function of VAP\_TEMP (°C)
- MSC\_TEMP(J) = temperature of boiling massecuite (°C), as mentioned in Section 10(a).
- STEAM\_TEMP = temperature of the heating vapour (°C), which could be a primary unknown when run in the Design or the Operation mode.

Equation (3) is only applied to compartments for which the amount of dilution water WASH(J) is known.

The equation can be used in the following ways:

- (a) HTC's and AREA's given: This is for the Operation mode.
- (b) HTC's unknown, AREA's given: This is for the Evaluation mode, where the HTC is assumed to be a linear function of the compartment index J, with the primary unknowns slope K\_UM and intercept K\_UB as parameters.
- (c) HTC's given, AREA's unknown: This is for the Design mode. AREA(J) is specified as proportional to primary unknown CELL\_VOL(J), and can thus be calculated.

**11. Setting up equations on the overall pan**

Of these equations there can be at most only one of each.

- Overall Syrup Feed balance:  $SOLIDS(N) - SOLIDS(0) = (Given) TOT\_SYRUP * (Given) SYRUP\_BX/100$
- Pan Exhaustion:  $XTAL(N)/SUC(N) = (Given) PAN\_EXH/100$
- Overall Calandria Condensate balance:

$$(3.6/LAT\_HT(STEAM\_TEMP)) \sum_{J=1}^N (STEAM\_TEMP - MSC\_TEMP) * (AREA(J) * HTC(J)) = (Given) CONDENSATE$$

This relationship is likely to arise in the Evaluation mode, when HTC as well as BPE will be functions of the primary unknowns. This will make the equation non-linear in the primary unknowns, so that it will also be part of the Newton-Raphson method, similar to the equations described in Section 10.

**12. Solution of the equations**

For a pan with 12 compartments, and the mainstreams therefore indexed 0 - 12, there will be about 56 primary unknowns. When in the Design or Operation mode, the number of equations should exactly equal the number of primary unknowns, so that the equations of each iteration can be solved directly. When in the Evaluation mode, there will usually be more equations than unknowns because of deliberate over-specification, and the program will first calculate the cross-product matrices as part of the linear regression fitting procedure and then perform the solution of simultaneous linear equations. In another publication Hoekstra<sup>6</sup> explains the principle behind this application of multiple linear regression analysis.

The simultaneous linear equations are solved by the Gaussian elimination procedure. The size of the matrix of coefficients and being in double precision, make it too large for the computer memory, and instead it is stored on disc in a record direct access file. Each time the program sets up an equation, its coefficients are written to file. During the course of the solution procedure, the relevant row is read from file, the necessary manipulations done on it, and written back to the disc file.

Because the iterative Newton-Raphson method of solution is used, the whole procedure of setting up and solving the equations has to be repeated several times. To indicate how far the process has converged, the intermediate results can be printed out after each iteration. To assist in tracing errors, the user can also request the entire matrix of coefficients of the equations to be printed out.

**13. Input and Output**

The input data to the program is in the form of a stream sequential file of a standard format, which the user fills in via the keyboard. The file format provides prompts and other indicators. The data is in free-format, meaning that an item does not have to be positioned exactly within certain columns on the screen. Where a data item is not known, the user inputs a 0 which the program interprets as "no data given" and will therefore not set up an equation for it. The file must also be given initial estimates of the primary unknowns, which are required to start off the Newton-Raphson method.

For the convenience of the user, CORPSE reproduces the abovementioned input to the computer in the same format as the final output, but shows values only for the given data items — the rest are not shown as zeros, but as blank spaces.

Figure 3 and Figure 4 respectively show a typical input and output of a run.

**14. Comments on the results**

When in the Evaluation mode and applying the least squares fit, many of the final results might not be quite the same as their corresponding values in the input data. This will be because they are back-calculated from the values of the primary unknowns which were solved in the final iteration, and will be

CONTINUOUSLY OPERATING RAW PAN SIMULATION AND EVALUATION ( C.O.R.P.S.E. )

DATE:27MAR85

TIME: 17:14:45

RUN NO: 26\_10\_2 MILL: MAIDSTONE OBJECT: A-PAN TRAILS: EVAL.OF 26/10/83, SHIFT 08 - 16.

SUMMARY OF INPUT DATA.

OVERALL PAN.

NO. OF COMPARTMENTS (N): 12 PAN EXHAUSTN:  
 MOLASSES OR SYRUP FEEDS: SOLIDS % SOLUTION : 67.3 PURITY (%) : 83.3 MASS (TONS/HR): 44.2  
 HEATING STEAM TO PAN : PRESSURE(kPa ABS.): 93.0 TEMPERATURE(DEG.C): 97.6 MASS (TONS/HR): 26.0  
 VAPOUR ABOVE PAN : PRESSURE(kPa ABS.): 15.0 TEMPERATURE(DEG.C): 54.0 MASS (TONS/HR):

PARAMETERS OF PAN: NO.OF XTALS (#1E+9) : 75.00 EMPIRICAL EQUATIONS: HTC(J) = -0.010 #J  
 GROWTH (K.GROWTH) : DISTR\_PARAM(J) = -0.080\*(J-6) + 4.074  
 SOLUBILITY (K\_SOLUB): 1.00 ASSUMED GRAIN SIZE DISTRIBUTION: GENERALISED NEGATIVE EXPONENTIAL

MASSECUITE STREAMS.

STREAM REF.NO.:	0	1	2	3	4	5	6	7	8	9	10	11	12
MASS RATES(TONS/HR):													
TOTAL MASS :													
SOLIDS :													
SUCROSE(INCL.XTAL:													
WATER :													
XTAL :													
VOL.FLOWRATE,CU.M/H:													
XTAL SIZES (MM) :													
BY MASS FREQ: MA :	.437	.456	.478		.554		.530		.582		.602		.604
BY NR. FREQ: L1 :	.237	.246	.256		.294		.279		.302		.309		.305
MASSEGU.PROPERTIES :													
SOLIDSXMASS<BRIX>:	86.80	89.00	88.70		88.80		89.00		89.00		89.10		89.60
SUCROSEXMASS<POL>:	73.60	75.90	75.40		75.30		75.50		75.30		75.10		76.10
PURITY (%) :													
XTAL % SOLIDS :													
DENSITY (GM/CC) :													
MOLASSES PROPERTIES:													
SOLIDSXMASS<BRIX>:	78.20	80.20	80.00		80.50		80.30		80.20		80.60		80.90
SUCROSEXMASS<POL>:	57.90	57.80	57.90		58.40		57.60		58.00		57.60		54.60
PURITY % <NUTSCH>:													
SUPERSATN (FRACN):													
IMPUR/WATER RATIO:													

COMPARTMENTS.

COMPARTMENT REF.NO.:	1	2	3	4	5	6	7	8	9	10	11	12
SPACE DETAILS :												
VOLUME (CU.M.) :	9.70	9.70	9.70	9.70	9.70	9.70	9.70	9.70	9.70	9.70	9.70	9.70
DEAD VOL.(FRACTN):												
RETENTION (HRS.) :												
CONTENTS PROPERTIES:												
GROWTH RATE(MM/H):												
HSC TEMP.(DEG.C.):												
MASS RATES(TONS/HR):												
SYRUP FEEDS :	0.00					0.00				0.00	0.00	0.00
MOVEMENT WATER :		0.00	0.00	0.00	0.00		0.00	0.00	0.00			
EVAPORATION :												
HEAT TRANSFER :												
HEAT TR.AREA, SQ.M:	91.0	91.0	91.0	91.0	91.0	91.0	91.0	91.0	91.0	91.0	91.0	91.0
H.T.C., KM/SQ.M-C :												
HEAT TR., KW :												

FIGURE 3 Input data to a CORPSE run in Evaluation mode.

CONTINUOUSLY OPERATING RAW PAN SIMULATION AND EVALUATION ( C.O.R.P.S.E. )

DATE:27MAR85

TIME: 17:49:04

RUN NO: 26\_10\_2 MILL: MAIDSTONE OBJECT: A-PAN TRAILS: EVAL.OF 26/10/83, SHIFT 08 - 16.

RESULTS OF RUN. ITERATION 6 OF 6 56 UNKNOWNNS, 90 RELATIONSHIPS.

OVERALL PAN.

NO. OF COMPARTMENTS (N): 12 STD.DEV.OF RES. OF PREV. ITERATION = 0.128 TONS/H PAN EXHAUSTN: 59.5  
 MOLASSES OR SYRUP FEEDS: SOLIDS % SOLUTION : 67.3 PURITY (%) : 83.3 MASS (TONS/HR): 43.6  
 HEATING STEAM TO PAN : PRESSURE(kPa ABS.): 93.0 TEMPERATURE( DEG.C): 97.6 MASS (TONS/HR): 25.7  
 VAPOUR ABOVE PAN : PRESSURE(kPa ABS.): 15.0 TEMPERATURE( DEG.C): 54.0 MASS (TONS/HR): 24.4

PARAMETERS OF PAN: NO.OF XTALS (\*1E+9) : 211.84 EMPIRICAL EQUATIONS:  $HTC(J) = -0.010 * J + 0.480$   
 GROWTH (K\_GROWTH) : .82841 DISTR\_PARAM(J) =  $-0.080*(J-6) + 4.074$   
 SOLUBILITY (K\_SOLUB): 1.00 ASSUMED GRAIN SIZE DISTRIBUTION: GENERALISED NEGATIVE EXPONENTIAL

MASSECUITE STREAMS.

STREAM REF.NO.:	0	1	2	3	4	5	6	7	8	9	10	11	12
MASS RATES(TONS/HR):													
TOTAL MASS :	24.29	24.01	30.63	37.00	42.01	41.91	42.66	46.55	51.19	56.52	56.44	56.07	56.29
SOLIDS :	21.09	21.40	27.17	32.72	37.31	38.09	37.96	41.52	45.54	50.30	50.27	50.34	50.42
SUCROSE(INCL.XTAL):	18.16	18.58	23.45	28.44	32.05	32.33	32.38	35.55	38.92	42.72	42.65	42.36	42.27
WATER :	3.20	2.61	3.46	4.28	4.70	3.82	4.70	5.03	5.65	6.22	6.17	5.73	5.87
XTAL :	9.80	11.41	13.48	15.92	18.17	18.34	18.68	20.39	22.14	23.17	24.16	24.67	25.17
VOL.FLOWRATE,CU.M/H:	16.78	16.39	20.96	25.35	28.72	28.35	29.14	31.77	34.98	38.61	38.54	38.15	38.34
XTAL SIZES (MM) :													
BY MASS FREQ: MA :	.431	.455	.482	.511	.535	.539	.544	.562	.580	.591	.601	.608	.615
BY NR. FREQ: LI :	.233	.245	.259	.273	.284	.285	.286	.294	.301	.305	.309	.310	.311
MASSECU. PROPERTIES :													
SOLIDS%MASS<BRIX>:	86.84	89.13	88.70	88.44	88.81	90.87	88.99	89.19	88.96	88.99	89.06	89.77	89.57
SUCROSE%MASS<POL>:	74.78	77.36	76.57	76.86	76.31	77.14	75.91	76.36	76.02	75.59	75.56	75.55	75.09
PURITY (%) :	86.12	86.79	86.33	86.91	85.92	84.89	85.31	85.61	85.46	84.94	84.84	84.16	83.83
XTAL % SOLIDS :	46.45	53.30	49.61	48.65	48.69	48.15	49.21	49.11	48.62	46.07	48.07	49.01	49.92
DENSITY (GM/CC) :	1.45	1.46	1.46	1.46	1.46	1.48	1.46	1.47	1.46	1.46	1.46	1.47	1.47
MOLASSES PROPERTIES:													
SOLIDS%MASS<BRIX>:	77.94	79.29	79.81	79.71	80.28	83.78	80.40	80.77	80.54	81.35	80.87	81.74	81.14
SUCROSE%MASS<POL>:	57.73	56.87	58.17	59.40	58.25	59.37	57.14	57.94	57.75	58.63	57.26	56.34	54.95
PURITY % <NUTSCH>:	74.07	71.72	72.88	74.52	72.56	70.86	71.07	71.73	71.70	72.07	70.80	68.93	67.72
SUPERSATN (FRACN):	.98	1.04	1.09	1.10	1.12	1.41	1.11	1.14	1.13	1.19	1.14	1.19	1.12
IMPUR/WATER RATIO:	.92	1.08	1.07	1.00	1.12	1.50	1.19	1.19	1.17	1.22	1.23	1.39	1.39

COMPARTMENTS.

COMPARTMENT REF.NO.:	1	2	3	4	5	6	7	8	9	10	11	12
SPACE DETAILS :												
VOLUME (CU.M.) :	9.70	9.70	9.70	9.70	9.70	9.70	9.70	9.70	9.70	9.70	9.70	9.70
DEAD VOL.(FRACTN):												
RETENTION (HRS.) :	.592	.463	.383	.338	.342	.333	.305	.277	.251	.252	.254	.253
CONTENTS PROPERTIES:												
GROWTH RATE(MM/H):	.022	.022	.025	.021	.012	.019	.019	.019	.018	.017	.014	.014
MSC TEMP.( DEG.C.):	61.4	61.5	61.4	61.7	63.4	61.8	61.9	61.9	62.2	62.0	62.5	62.3
MASS RATES(TONS/HR):												
SYRUP FEEDS :	.46	8.57	8.25	6.81	1.16	-.19	5.30	5.97	7.07	-.04	.11	.13
MOVEMENT WATER :	1.60	.33	.36	.37	.76	3.00	.61	.64	.15	1.83	1.31	1.84
EVAPORATION :	2.34	2.28	2.24	2.17	2.02	2.06	2.01	1.96	1.90	1.86	1.78	1.75
HEAT TRANSFER :												
HEAT TR.AREA, SQ.M:	91.0	91.0	91.0	91.0	91.0	91.0	91.0	91.0	91.0	91.0	91.0	91.0
H.T.C., KW/SQ.M-C :	.470	.460	.450	.440	.430	.420	.410	.400	.390	.380	.370	.360
HEAT TR., KW :	1548.8	1509.8	1481.5	1436.4	1336.1	1366.6	1329.6	1300.6	1256.6	1229.3	1180.9	1155.7

FIGURE 4 Results from a CORPSE run.



somewhere "in-between" the over-specified input data, in the same way that a least-squares fit of a straight line to a number of points will not, in general, pass directly through any one of the points.

As an example, part of the results of a series of 6 tests which were taken on each of 3 shifts on 26 and 27 October 1983 on a continuous A-pan at Maidstone and subsequently run on CORPSE in the Evaluation mode are shown:

Date:	26.10.83			27.10.83		
Shift:	1	2	3	1	2	3

*Growth rate constant*

K\_GROWTH (mm/h): 0.835 0.828 0.646 0.865 0.885 0.521

*Heat transfer coefficient (kW/(m<sup>2</sup>C)):*

HTC of Compartment 1: 0.472 0.470 0.478 0.392 0.400 0.456

HTC of Compartment

12: 0.362 0.362 0.368 0.282 0.290 0.346

*Common supersaturation:*

K\_SUPERSATN 1.20 1.17 1.16 1.19 1.21 1.26

Considering the practical problems in measuring some of the flow rates accurately and in obtaining representative samples from the compartments of a plant which has a long hold-up time, the above variations in results seem reasonable.

The following remarks apply:

*Growth rate constant*

The growth rate constant in the formula proposed by Wright<sup>14</sup> is 7.418 mm/h, which is higher than that obtained here by a factor of about 10. This could be due to the many assumptions and simplifications which have had to be made in the computerised model, compared with the rigorous analysis by Wright.

*Heat transfer coefficients*

Because the factory installations on which the evaluations were performed thus far had no facilities for measuring the amounts of syrup and dilution water going into individual compartments, except of course where the amount was zero, it was not feasible for CORPSE to calculate a heat transfer coefficient for each compartment separately. To use the same value of heat transfer coefficient for all compartments would be too severe an approximation, and it was decided to let the HTC decrease in a linear manner from the first to the last compartment. The rate of decrease was estimated for a 12-compartment pan to be 0.01kW/(m<sup>2</sup>C) per compartment, and was specified as an input for the slope K\_UM of the line, so that CORPSE then merely had to calculate the intercept K\_UB of the line.

*Supersaturation*

Each supersaturation value given in the table is the solution to the primary unknown K\_SUPERSATN which is taken to be common for all compartments, per Section 10(b). They are generally at the level one would expect. When re-calculating it back for individual compartments J from the applicable mass values SOLIDS(J), SUC(J), WATER(J) and XTAL(J), there is considerable variation amongst compartments, as can be seen in Figure 4.

## 15. The Computer

The computer used is a Data General Eclipse S/140 with 3/4 Megabyte of memory and 75 Megabyte of disc storage. It operates under the Data General Advanced Operating System, and the program was written in the language PL/1. Because of its size, the program had to be broken up into smaller procedures, and overlays used.

When in the Evaluation mode, 6 iterations are usually required, which require about 40 minutes of run time for a 12-compartment pan. In the Design or Operation mode 3 itera-

tions often suffice, and the run time is down to about 15 minutes because of this and because no-least-squares fit is required.

## 16. Concluding Remarks

CORPSE makes no pretence at being a rigorous model of the basic principles of sucrose crystallisation. It must be considered as a tool to be used not only for comparing the relative performances of different continuous pans when in the Evaluation mode, but also for applying the empirically obtained process parameters of growth rate constant and heat transfer coefficients to simulation purposes when in the Design or Operation mode. The previously mentioned self-compensating effect of errors resulting from certain assumptions or simplifications would apply, among others, to grain size distributions and their changes from compartment to compartment, the cubic shape of the crystals, the growth rate independence of crystal size, constancy in the number of crystals, the zero dead volume per compartment and the impurity effects on mass transfer.

## 17. Acknowledgement

I want to pay tribute to Dr Ross Broadfoot<sup>3</sup> for his Ph.D. thesis on continuous crystallisers. The orderly way in which he discussed the relationships was a great help in the writing of the program.

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## APPENDIX 1

### GENERALISED NEGATIVE EXPONENTIAL PROBABILITY DENSITY FUNCTION

The probability density function (p.d.f.) for the size-frequency-by-number distribution is:

$$f(x) = \frac{p}{k} \cdot \frac{\exp(-(x/k)^p)}{\Gamma(1/p)}$$

where  $x$  = size (length),  $> 0$

$p$  = shape parameter,  $> 0$ , dimensionless

$k$  = scale parameter,  $> 0$ , with same dimension as  $x$

$\Gamma(r)$  = Gamma function with parameter  $r$

$$= \int_0^{\infty} t^{r-1} e^{-t} dt, \text{ for } r > 0$$

=  $(r-1)!$  for  $r$  a positive integer.

The corresponding cumulative distribution function (c.d.f.), which is used in determining the parameters p and k by fitting to experimental results of grain counting, is obtained by putting  $t = (x/k)^p$  in the above equation and integrating:

$$\begin{aligned} & \text{Probability (Randomly selected grain size } \leq x) \\ & = F(x) \\ & = \int_0^{(x/k)^p} \frac{t^{(1/p) - 1} e^{-t}}{\Gamma(1/p)} dt \end{aligned}$$

The mean-size-by-number is obtained from:

$$\begin{aligned} L_1 & = \int_0^\infty x f(x) dx \\ & = k\Gamma(2/p)/\Gamma(1/p) \end{aligned}$$

The p.d.f. for the size-frequency-by-mass is given by:

$$\begin{aligned} g(x) & \equiv \frac{\int_0^x t^3 f(t) dt}{\int_0^\infty t^3 f(t) dt} \\ & = \frac{p}{k} \cdot \left(\frac{x}{k}\right)^3 \frac{\exp(-(x/k)^p)}{\Gamma(4/p)} \end{aligned}$$

and the corresponding c.d.f. by:

$$G(x) \equiv \int_0^{(x/k)^p} \frac{t^{(4/p) - 1} e^{-t}}{\Gamma(4/p)} dt$$

The mean-size-by-mass is obtained from:

$$\begin{aligned} MA & = \int_0^\infty xg(x) dx \\ & = k\Gamma(5/p)/\Gamma(4/p) \end{aligned}$$

It can similarly also be shown that mean-volume-by-number

$$\begin{aligned} V & = \int_0^\infty x^3 f(x) dx \\ & = k^3\Gamma(4/p)/\Gamma(1/p) \end{aligned}$$

This gives the relationships which are required in the running of CORPSE:

$$\begin{aligned} VL3 & = V/L_1^3 \\ & = \frac{\Gamma(4/p)(\Gamma(1/p))^2}{(\Gamma(2/p))^3} \end{aligned}$$

$$\text{and } MA/L_1 = \frac{\Gamma(5/p) \Gamma(1/p)}{\Gamma(2/p) \Gamma(4/p)}$$

Note that the scale parameter k cancels out, so that these relationships are only a function of the shape parameter p.

## APPENDIX 2

### DERIVATION OF EMPIRICAL EXPRESSION FOR BOILING POINT ELEVATION OF CONCENTRATED SUGAR SOLUTIONS

The task was to derive an empirical relationship for boiling point elevation (BPE) in terms of the concentration of the mother liquor (molasses), the boiling point of pure water at the particular vapour space operating pressure and the degree of impurity, by applying multiple linear regression analysis to tabular data.

From thermodynamic principles, the following relationship can be approximated for pure, dilute solutions from the Gibbs-Helmholtz equation (see Moore<sup>11</sup>):

$$BPE = \frac{K m_B T^2}{m_A}$$

where K = constant

$m_B$  = mass of solute

$m_A$  = mass of solvent

T = boiling point of pure solvent, °K

This suggested using the form

$$BPE = AO*(S\_W\_RATIO)^{A1} * (T\_ABS)^{A2}$$

where S\_W\_RATIO = Solids-to-Water ratio of mother liquor

$$= \frac{SOLIDS(J) - XTAL(J)}{WATER(J)}$$

T\_ABS = Absolute temp. of pan vapour

AO, A1 and A2 = Regression constants

In a pure, dilute solution one should expect that A1 = 1 and A2 = 2, but letting them find their own best-fit level would help compensate for non-ideality.

Impurity of the mother liquor was brought into account by the additional product term (NUTSCH\_PUR)<sup>A3</sup>

where NUTSCH\_PUR = Purity of mother liquor (as a fraction)

$$= \frac{SUC(J) - XTAL(J)}{SOLIDS(J) - XTAL(J)}$$

A3 = Regression constant.

Note that, for a pure solution, this term = 1, whatever the value of A3.

By taking logs, the entire equation could be linearised for regression analysis purposes:

$$\ln BPE = \ln AO + A1 * \ln(S\_W\_RATIO) + A2 * \ln(T\_ABS) + A3 * \ln(NUTSCH\_PUR)$$

Data from Honig<sup>7</sup>, which dealt with comparatively pure solutions, was used to determine the constants AO, A1 and A2. Data from Batterham & Norgate<sup>2</sup>, Hugot<sup>8</sup> and Lyle<sup>10</sup> was used to determine A3.

The final equation obtained was:

$$BPE = 0.1379 * (S\_W\_RATIO)^{0.808} * (T\_ABS)^{2.327} * (NUTSCH\_PUR)^{-0.42}$$