Computer Method for Calculating Percentage Apparent Purity of Sugar Beet Thin Juice[1]

GEORGE A. MILLIKEN AND RICHARD J. HECKER[2]

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The percentage apparent purity of sugar beet thin juice is used to determine the processing quality of sugar beets. Because of the increasing importance of purity, sugar beet breeders are carrying out more extensive research programs on this character. The apparent thin juice purity is ordinarily determined on sugar beet pressed juice which has been defecated with lime, then partially neutralized with oxalic or phosphoric acid. This thin juice closely approximates the factory second carbonation juice, Carruthers and Oldfield (3)[3]. This calculation of percentage thin juice purity from the thin juice saccharimeter and refractometer readings is a time-consuming and costly operation when done manually. Hence a method was developed to compute this apparent purity on an electronic computer. A computer is designed to do routine calculations, such as this, with high speed and accuracy, resulting in lower computation costs and elimination of human error in the calculating and checking processes.

The purity of a sugar solution may be defined as the percentage of total solids (dry substance) of the solution which is sugar, as expressed in the simple formula:

$$\text{PURITY} = \frac{\text{percent sucrose}}{\text{percent solids}} \times (100) \qquad [1]$$

The method for purity determination of thin juice, according to Brown and Serro (2) as modified by Carruthers and Oldfield (3), employs a refractometer and a saccharimeter. The refractometer provides the refractive index and the saccharimeter provides the polorization of the thin juice based on the International Sugar Scale. Because the thin juice is an impure solution, and the above two readings are based on the refractive index and

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[2] Graduate Fellow, Department of Mathematics and Statistics, Colorado State University, and Research Geneticist, Crops Research Division, Agricultural Research Service, U. S. Department of Agriculture, Fort Collins, Colorado.

[3] Numbers in parentheses refer to literature cited.

saccharimeter readings of a pure sucrose solution, the laboratory determination is called "apparent purity".

In the normal process of purity determination a sample of thin juice is placed in a precision refractometer and a reading is taken. The refractive dry substance (RDS), or total soluble matter in an impure sugar solution, corresponding to the refractive index, is read from the refractometer conversion tables. Each refractometer instrument has its own set of RDS conversion tables which depend upon the calibration of the instrument. Thus the statements in this paper concerning the refractometer tables are for the Bausch and Lomb precision refractometer used at the Sugarbeet Investigation Laboratory, Crops Research Division, U. S. Department of Agriculture, Fort Collins, Colorado. The remaining thin juice is then poured into the saccharimeter (200 mm tube) to obtain the polarization on the International Sugar Scale.

Using the RDS and the saccharimeter reading the apparent purity is calculated by

$$\text{APPARENT PURITY} = \text{FACTOR} \times \text{SACCHARIMETER READING} \qquad [2]$$

where the factor is determined by

$$\text{FACTOR} = \frac{26.00}{0.99717 \times \text{sp gr} \times \text{Brix}} \qquad [3]$$

where: 26.00 is the "normal weight" for sucrose, [Bates (1) p. 79]; 0.99717 is the apparent density of water at 20°C [Bates (1) p. 632]; and sp gr is the specific gravity of water at 20°/20°C for the Brix of the solution. Brix in this case is RDS.

Consider a sample of thin juice with a saccharimeter reading of 40.3 and a refractive index of 24.29. The RDS corresponding to this refractometer reading is obtained from the refractometer conversion tables and is read to be 11.70. The specific gravity corresponding to this RDS (or Brix) is 1.04706 [see Bates (1) pp. 614-623]. Thus, the factor is:

$$\text{FACTOR} = \frac{26.00}{(0.99717)\ (1.04706)\ (11.70)} = 2.1284.$$

The apparent purity is then:

$$\text{APPARENT PURITY} = (2.1284)\ (40.3) = 85.77.$$

An instrument called a "purity wheel" has been constructed in the form of a circular slide rule where the scales are such that when the RDS and saccharimeter readings are lined up the apparent purity is calculated, taking into account the specific gravity corresponding to the given RDS. Thus, in effect, one scale corresponds to the values of the factor and the combination of the scales carries out the multiplication of the factor and the saccharimeter reading. The purity wheel is probably the most frequently used method for calculating percentage apparent purity. There are two weak points in using the purity wheel. First, the purity wheel is not finely scaled. For example, if the RDS is 11.73, it would be hard to locate exactly the position of the hairline, which could result in a purity error as high as 0.2 percent. Second, the purity wheel is not constructed such that low values of RDS (below 8.0) can be used. A set of tables has been calculated to handle these lower values, but they are in increments of 0.05 units on the RDS scale. If one has an RDS of 7.38, he would have to interpolate between 7.35 and 7.40, or he would use the purity value corresponding to the RDS of 7.40. Most interpolations are carried out on a linear basis and it could bias the results since the proper interpolation is not linear in form.

One method of calculating the apparent purity on a computer directly from the refractometer reading and the saccharimeter reading, would be to enter the refractometer conversion tables and the specific gravity tables into the computer. From this the computer could be programmed to call from storage the RDS value corresponding to the refractometer reading and then recall the specific gravity corresponding to the RDS of the solution. The apparent purity could then be calculated, using equations [2] and [3]. However, this is not a feasible method, since these tables are very large and the average computer is not big enough to store the tables and the program needed to do the calculations. Thus the computer method which we have developed for calculating the percentage apparent purity consists of programming the computer to obtain an equation which approximates the refractometer conversion tables; i.e., given a refractometer reading, the equation gives the RDS value. The computer was also programmed to obtain a second equation which approximates the FACTOR (equation [3]); i.e., given the RDS value, the equation gives the corresponding factor. Then the computer is programmed to use these two equations to obtain the factor and to multiply the factor and saccharimeter reading to obtain the apparent purity.

Specifically a computer is used to determine an accurate equation to approximate the refractometer conversion tables furnished with the refractometer (Table 1, columns 1 and 2). The process consists of fitting a polynomial equation to the refractometer readings (scale) and the corresponding RDS values by using a standard polynomial fit computer program. The particular program used generates five equations, linear through a fifth degree polynomial. For each equation, the program expresses the goodness of fit by calculating the coefficient of determination (R^2).

Table 1.—Comparison of tabular and computer calculated refractive dry substance values, using equation [4].

Refractometer reading	Tabular RDS[1]	Computed RDS
21.50	1.70	1.72
22.00	3.58	3.59
22.50	5.42	5.41
23.00	7.22	7.21
23.50	8.98	8.97
24.00	10.71	10.71
24.50	12.41	12.40
25.00	14.07	14.07
25.50	15.70	15.70
26.00	17.29	17.30
26.50	18.86	18.87
27.00	20.39	20.40
27.50	21.90	21.90
28.00	23.38	23.37

[1] These RDS values are from the conversion tables furnished with the Bausch and Lomb precision refractometer at Sugarbeet Investigations, Fort Collins, Colorado.

The equation chosen to approximate our set of conversion tables was:

$$RDS = -109.4991 + 6.58860\,(REF) - 0.065836\,(REF)^2 \quad [4]$$

where REF = refractometer reading.

The quadratic equation was chosen because its R^2 value is 0.9999. Thus the approximation could not be improved by using a higher degree polynomial. Conversion tables for other refractometers may be best approximated by a higher degree polynomial.

The next step was to obtain the equation from which the factor can be calculated by using the RDS calculated above. A table of factors was calculated by Rice (4), using equation [3], the factors being wholly determined by the RDS. The graph of the table (RDS vs. FACTOR) is hyperbolic in form (the form $y = a/x$). Thus in order to use the polynomial fit program, the points in the factor table (1, 25.9725; 2, 12.9360; etc.; see Table 2) were transformed by multiplying each factor by the corresponding RDS. Polynomial equations were then fit to the transformed data (1, 25.9725; 2, 25.8720; etc.). The quadratic equation was chosen to approximate the transformed factor table, since its $R^2 = 0.9999$. The equation is:

$$\text{TRANSFORMED FACTOR} = 26.0731 - 0.100654(RDS) + 0.0000453\,(RDS)^2 \quad [5]$$

$$\text{FACTOR} = \text{TRANSFORMED FACTOR} \,/\, RDS. \quad [6]$$

Referring to the above example where the saccharimeter reading was 40.3 and the refractometer reading 24.29, let us calculate percentage apparent purity, using the above equations, thus, simulating the computer method.

$$\begin{aligned} RDS &= -109.4991 + (6.58860)(24.29) - (0.065836)(24.29)^2 \\ &= -109.4991 + 160.0371 - 38.8435 \\ &= 11.6945 \end{aligned}$$

$$\begin{aligned} \text{TRANSFORMED FACTOR} &= 26.0731 - (0.100654)(11.6945) + (0.0000453)(11.6945)^2 \\ &= 26.0731 - 1.1771 + 0.0062 \\ &= 24.9022 \end{aligned}$$

$$\text{FACTOR} = 24.9022 / 11.6945 = 2.1294$$

$$\text{APPARENT PURITY} = (2.1294)(40.3) = 85.81$$

If the calculations were carried out on a calculator, the above equations would not be practical to use, whereas a computer can utilize them very efficiently.

To show how accurate the approximations are, portions of Tables 1, 2, and 3 were generated by using equation [4] and

Table 2.—Approximated factors for purity computed from saccharimeter reading and dry substance, and purity factors [from Rice (4)].

Dry substance (RDS) or Brix	Computed factor	Factors from Rice (4)
1	25.9725	25.9725
2	12.9360	12.9360
3	8.5905	8.5905
4	6.4178	6.4178
5	5.1142	5.1142
6	4.2451	4.2451
7	3.6244	3.6244
8	3.1588	3.1589
9	2.7968	2.7968
10	2.5071	2.5071
11	2.2701	2.2701
12	2.0726	2.0727
13	1.9056	1.9056
14	1.7624	1.7623
15	1.6382	1.6382
16	1.5296	1.5296
17	1.4338	1.4338
18	1.3487	1.3487
19	1.2725	1.2725
20	1.2039	1.2039
21	1.1419	1.1419
22	1.0855	1.0855
23	1.0340	1.0340
24	0.9868	0.9868

equations [5] and [6]. Columns 1 and 2 of Table 1 are a segment of the conversion table used to calculate purity the manual way, and column 3 was generated from equation [4]. Comparisons of the tabular RDS values and the computed RDS values show deviations of at most 0.02 RDS units. A segment of the table of computed factors is shown in Table 2 and it compares almost identically (to 0.0001) to the factors produced by Rice (4). Table 3 is a check of the accuracy of the method and contains 40 purity calculations from actual data. These

Table 3.—Comparison of computer calculations with tubular dry stubstances and hand calculated apparent purities.

Sacharimeter reading	Refractometer reading	Tubular dry substance	Computer calculated dry substance	Apparent purity	Purity wheel calculated purity	Computer calculated purity
40.50	23.95	10.54	10.53	96.13	96.10	96.19
42.70	24.33	11.83	11.83	89.84	89.70	89.84
42.10	24.05	10.88	10.88	96.67	96.70	96.70
43.60	24.15	11.22	11.22	96.95	97.00	96.97
35.80	23.57	9.22	9.22	97.65	97.70	97.66
42.40	24.17	11.29	11.29	93.67	93.80	93.70
43.00	24.13	11.15	11.15	96.24	96.30	96.24
44.60	24.22	11.46	11.46	97.01	97.00	97.04
42.30	24.12	11.12	11.12	94.95	94.90	94.98
41.50	24.00	10.71	10.71	96.87	96.90	96.92
38.50	23.93	10.47	10.47	92.02	92.10	92.06
19.50	22.43	5.16	5.16	96.57	96.50	96.56
42.50	24.14	11.19	11.18	94.77	94.80	94.82
50.50	24.70	13.07	13.07	95.69	95.80	95.66
50.50	24.64	12.87	12.87	97.25	97.40	97.23
44.20	24.25	11.56	11.56	95.26	95.30	95.28
44.80	24.15	11.22	11.22	99.62	99.60	99.64
40.30	24.29	11.70	11.69	85.77	85.70	85.82
46.70	24.40	12.07	12.07	96.21	96.30	96.23
45.40	24.34	11.87	11.86	95.18	95.30	95.23
44.40	24.28	11.66	11.66	94.85	94.90	94.84
45.70	24.36	11.93	11.93	95.30	95.30	95.29
36.70	23.68	9.60	9.60	96.00	96.00	95.98
41.10	24.06	10.91	10.91	94.11	94.10	94.10
47.80	24.52	12.48	12.47	95.08	95.10	95.16
41.50	23.97	10.61	10.60	97.82	97.80	97.90
44.00	24.24	11.53	11.52	95.09	95.00	95.14
41.60	24.03	10.81	10.81	96.17	96.20	96.19
41.00	23.99	10.68	10.67	95.99	96.00	96.07
42.70	24.17	11.29	11.29	94.34	94.40	94.37
35.90	23.69	9.64	9.64	93.50	93.50	93.54
46.60	24.40	12.07	12.07	96.00	96.10	96.03
40.50	23.94	10.51	10.50	96.41	96.40	96.51
40.60	23.90	10.37	10.36	98.01	98.10	98.09
41.50	24.04	10.85	10.84	95.57	95.60	95.64
43.30	24.18	11.32	11.32	95.40	95.40	95.39
46.80	24.36	11.93	11.93	97.60	97.60	97.59
41.40	24.06	10.91	10.91	94.79	94.80	94.78
38.50	23.84	10.16	10.16	94.94	95.00	94.99
41.00	23.94	10.51	10.50	97.60	97.70	97.71

purities in column 5 are the actual apparent purities calculated by using equations [2] and [3]; those in column 6 were obtained on the purity wheel; those in column 7 were obtained by the computer, using equations [4], [5], and [6]. The calculation of the dry substance showed an average deviation of 0.003 RDS units and a standard error of 0.0007. These comparisons show a maximum deviation of 0.01, which is less error than can be accounted for by temperature control which should be held constant at 20°C when obtaining the refractometer reading. The computer calculation of apparent purity from the calculated dry substance showed an average deviation of 0.030 percent and a standard error of 0.0056 percent. The purities calculated on the purity wheel from the tabular RDS values showed an average deviation of 0.028 percent and a standard error of 0.0103. The standard error of the purity wheel calculations was twice that of the computer method. This shows how human error can enter into the calculation. By using the computer method, the interpolation is carried out in the proper form for the purities obtained when the dry substance becomes too small to use the purity wheel.

To use the computer method, one must first have an equation fit to the points (refractive index vs. RDS) of his refractometer conversion tables, since each refractometer has its own set of tables. If a programmer is not available to assist in obtaining an equation, take the conversion tables to a computer center where this equation can be generated. The type of equation needed is one which calculates the RDS value from a given refractive index. This is the only new equation required since the factor does not depend upon the refractometer used. Using this developed equation and equation [5], a program can now be written to calculate the percentage apparent purity. If the user is already doing analysis of variance or some other types of analyses on the apparent purity data, the above equations can be inserted into the program, thus computing the apparent purity before continuing with the analysis. Therefore the saccharimeter reading and the refractometer reading would be punched into the data cards instead of the apparent purity.

A scientific electronic computer with a high speed memory can compute the 40 apparent purities in Table 3 in less than one second. Even though computers are expensive to operate, the cost of making large numbers of purity calculations by computer is still much less than calculating and checking the purity determinations on a purity wheel. Moreover, the computer method is at least as accurate.

Summary

A computer method was developed to calculate the percentage apparent purity of sugar beet thin juice. These computations were made directly from the thin juice saccharimeter and refractometer readings.

First the refractive dry substance values (specific for each refractometer) and a table of factors were approximated by using a polynomial fit computer program. A quadratic equation was satisfactory in each case. However, the quadratic equation approximating the refractive dry substance values would not necessarily be the best equation in every case. Percentage apparent purity was then computed directly from the refractive dry substance and the factor, using existing equations. The computer method was found to be at least as accurate as the purity wheel method of calculating apparent purity of sugar beet thin juice, but should be much more economic when many purity determinations are necessary.

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