USE OF CHEMICAL COMPOSITION OR NEAR INFRARED REFLECTANCE SPECTROSCOPY TO PREDICT THE GROSS ENERGY CONTENT OF CANE MOLASSES

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Story in Brief

Twenty-three samples of cane molasses were analyzed to evaluate the relationship between chemical composition and gross energy (GE; kcal/g) content. Ash content (%) was the best single predictor (R^2=.74) of gross energy. The best multiple regression equation included both dry matter (%) and ash (%): $GE = 505{,}792 - 19{,}332.16*DM + 247.842*DM^2 - 1.0581*DM^3 - .092*ASH^3$ (R^2=.86). Analysis of cane molasses samples with near infrared reflectance spectroscopy showed that gross energy could be predicted fairly accurately (R^2=.86). This study suggests that the gross energy content of cane molasses can be predicted with either a simple laboratory analysis (ash) or near infrared reflectance spectroscopy. Due to the small data base, however, further sample analyses and development of near infrared reflectance spectroscopy calibration equations should be completed prior to implementation of the technique.

(Key Words: Cane Molasses, Gross Energy, Near Infrared Reflectance Spectroscopy.)

Introduction

Cane molasses, a byproduct of the sugar refining industry, is one of the most common feedstuffs used in livestock diets. Its primary function is to reduce dust thereby enhancing palatability. The nutrient composition of molasses is affected by the variety and maturity of the cane as well as climatic and soil conditions during growth. In addition, plant refinement conditions and procedures can alter composition. Because of these inherent sources of variation, the energy content of molasses is not consistent. Therefore, the

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objective of this research was to evaluate laboratory procedures which could be used to predict the gross energy content of molasses.

Materials and Methods

Cane molasses samples (n=23) were obtained from various sources by Cargill's Molasses Division. Molasses samples were frozen, freeze dried, and ashed (500°C, 8 h) to determine their dry matter and ash content. Freeze drying was preferred over conventional oven drying (100°C, 24 h) to reduce volatilization of organic compounds by high temperature. Gross energy content was determined on non-dried samples with a Parr Oxygen-Bomb Calorimeter. Subsequent gross energy (GE) values (kcal/gram) were converted to a dry matter basis. Total sugars as invert (TSI), solids (S) and brix values were determined by a Cargill Laboratory and are expressed on a non-dried basis. Invert sugars are a measure of fructose content and solids are equivalent to dry matter content. Brix is the specific gravity of the molasses relative to solutions of known sucrose content. All independent variables were submitted to stepwise regression analysis to derive relationships between chemical constituents and GE. Multiple linear regression was used to determine the best multiple variable equation.

In addition, molasses samples were evaluated with near infrared reflectance spectroscopy (NIR) at the Southwest Livestock and Forage Research Laboratory located at El Reno, OK. Samples were scanned with near-infrared light (1100-2500 nm) and the reflected energy recorded at 2 nm intervals. Samples were placed in forage sample cups encased in polyethylene film. Although the film has a spectra, all samples were treated the same so the polyethylene peaks would be ignored in the regression for gross energy. Calibration equations were developed using a modified stepwise regression of gross energy on each of the 700 absorbance values across the spectrum.

Results and Discussion

Gross energy content of cane molasses averaged 3,447 kcal/g DM and was the least variable (CV=2.17) chemical component (Table 1). Ash content was the most variable chemical component (CV=11.53) followed by invert sugars (CV=7.82). Observed values for all chemical analyses were similar to reported values (Baker, undated).

The gross energy content (DM basis) of cane molasses was most highly correlated (r=-.85) with ash content expressed on a DM basis (Table 2). Ash dilutes energy density and should reduce gross energy content. A simpler analytical procedure would be to measure the ash content of wet molasses. The

Table 1. **Variation in chemical composition of cane molasses samples.**

Component	N	Range Minimum	Range Maximum	Mean	SD[a]	CV[b]
Gross energy, kcal/g DM	23	3294.3	3588.2	3447.2	74.82	2.17
Dry matter, %	23	72.5	82.3	78.6	3.54	4.50
Ash, % of DM	23	9.5	15.6	13.1	1.51	11.53
Invert sugars, % of as-is	23	44.8	57.5	50.9	3.98	7.82
Solids, % of as-is	23	69.9	83.5	76.5	3.32	4.34
Brix, degrees, as-is basis	23	79.8	87.7	84.5	2.73	3.23

[a] Standard deviation.
[b] Coefficient of variation (SD/mean x 100).

Table 2. Simple correlations between gross energy content and chemical components[a] of cane molasses.

	DM	ASH(DM)	ASH(AS-IS)	SOLIDS	TSI	BRIX
GE	.17 (.44)[b]	-.85 (.01)	-.77 (.01)	.17 (.43)	.35 (.10)	.05 (.82)
DM		-.30 (.16)	-.61 (.01)	.88 (.01)	.60 (.01)	.95 (.01)
ASH(DM)			.94 (.01)	-.27 (.21)	-.62 (.01)	-.10 (.64)
ASH(AS-IS)				-.54 (.01)	-.73 (.01)	-.42 (.04)
SOLIDS					.58 (.01)	.87 (.01)
TSI						.56 (.01)

[a] GE=gross energy (DM basis); DM=dry matter; ASH(DM)=ash (DM basis); ASH(AS-IS)=ash (as-is basis); SOLIDS=solids (as-is basis); TSI=total sugars as invert (as-is basis); BRIX=degrees brix (as-is basis).

[b] Simple correlation coefficient (probability value).

correlation between gross energy and as-is ash content was lower (r=-.77) than for ash content corrected for moisture. Common molasses analyses were poorly correlated (r=.17 for SOLIDS, r=.35 for TSI, r=.05 for BRIX) with gross energy. The brix scale relates the specific gravity of a sucrose solution to its sucrose content. Degrees brix, however, does not indicate the sugar content of molasses (Baker, undated). Consequently, the low correlation between brix and gross energy (r=.05) was expected. Brix (r=.95) and solids (r=.88) were highly correlated with molasses dry matter content.

Single component linear regression analysis showed that ash content (% of DM) was the single best predictor ($GE=3,999-42.21*ASH$; $R^2=.72$) of the gross energy content (kcal/g DM) of cane molasses (Figure 1). Simple linear regression using ash cubed ($GE=3,657-.091*ASH^3$) improved the relationship slightly ($R^2=.74$; Table 3).

Multiple regression was utilized to evaluate the predictive value of multiple chemical analyses for gross energy content (Table 3). Adding variables deemed significant ($P<.10$) increased the R^2 and decreased the mean square error (MSE). The equation with the highest correlation coefficient and lowest MSE utilized DM, DM^2, DM^3, and ASH^3.

The predictive value of NIR analysis for gross energy ($R^2=.86$) and brix values ($R^2=.86$) of cane molasses was high (Table 4). NIR predicted the dry matter, invert sugars and solids values with intermediate accuracy. The poorest

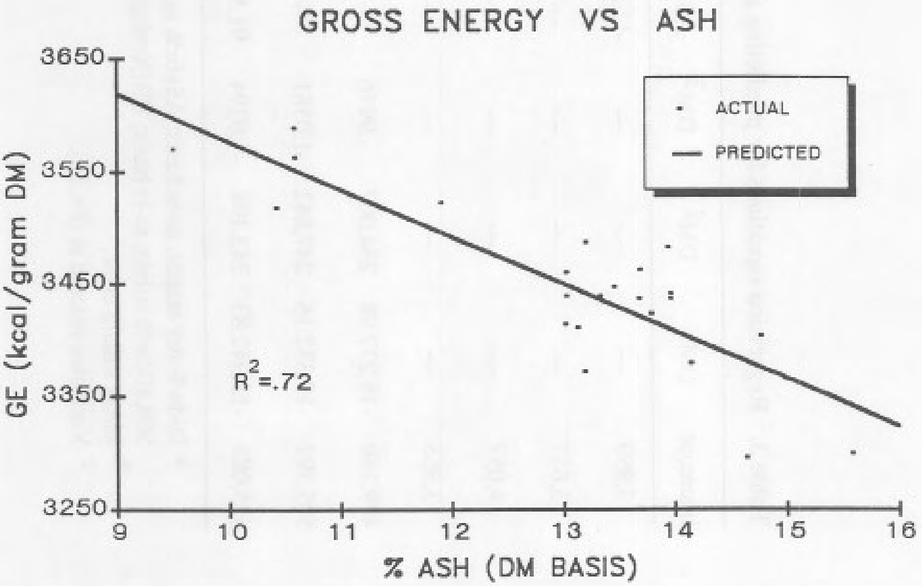

Figure 1. Relationship between the ash content of cane molasses and gross energy (GE).

Table 3. Regression equations for predicting gross energy from molasses chemical composition[a].

Intercept	DM	DM^2	DM^3	ASH	ASH^2	ASH^3	TSI	SOLIDS	BRIX	R^2	MSE[b]
3,999	---	---	---	-42.21	---	---	---	---	---	.72	1,616.3
3,657	---	---	---	---	---	-0.091	---	---	---	.74	1,495.0
4,057	---	---	---	---	-2.04	---	-5.05	---	---	.78	1,329.9
3,965	---	---	---	---	-2.06	---	-6.13	1.96[c]	---	.79	1,367.5
479,140	-18,277.98	234.007	-.9976	---	-1.74	---	---	---	---	.85	1,023.9
505,792	-19,332.16	247.842	-1.0581	---	---	-0.092	---	---	---	.86	956.2
495,085	-18,942.83	243.198	-1.0394	91.50[c]	-5.28	---	---	---	-9.36[c]	.87	981.9

[a] DM=% dry matter, as-is basis; ASH=% ash, DM basis; TSI=% total sugars as invert, as-is basis; SOLIDS=% solids, as-is basis; BRIX=degrees brix, as-is basis.

[b] Mean square error.

[c] Variables entered at ($P<.35$).

Table 4. Near infrared reflectance spectroscopy analysis of cane molasses samples.

Item	R^2	SEC[a]
Gross energy	.86	34.20
Dry matter	.76	1.68
Ash	.60	.97
Solids	.70	1.82
Invert sugars	.72	2.11
Brix	.86	1.05

[a] Standard error of calibration.

relationship was for ash (R^2=.60). Because the same 23 molasses samples were used to generate and to test the NIR calibration, the usefulness of these data are limited. The high coefficients of determination (R^2) suggest that NIR may be useful for cane molasses analysis.

These data indicate that the ash content of cane molasses is the best single predictor (R^2=.72) of gross energy content. A multiple regression equation using dry matter content combined with ash accounted for 86% of the variation in gross energy. But because the number of samples was small, the data from this study should be considered as preliminary. A larger data set should be evaluated to determine these relationships more precisely and to detect outliers.

Literature Cited

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