Utilization of Mathematical Models to Characterize Functional Properties of Selected Emulsifiers in Continuous Mix Bread

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ABSTRACT AND SUMMARY

Research conducted to determine the functional properties of food emulsifiers encompassed by the Bread Standards facilitated the development of mathematical models. Areas of functional utility are characterized by this mechanism. Emulsifiers were investigated individually and in combination with a complementary softener or conditioning agent. The evaluation resulted in classified functionality and ranked responses for specified areas of: (a) bread softness retention, (b) shock tolerance, and (c) specific bread volume. Mathematical techniques employed to describe the models consist of equations having the form:

$$\text{Functional Response} = \beta_{S_i}(\%\ S_i) + \beta_{C_j}(\%\ C_j) + \beta_{S_iC_j}(\%\ S_i)(\%\ C_j) \text{ where,}$$
$$S_i = \text{softener},\ C_j = \text{conditioner}.$$

Binary mixture experiments utilizing interaction modeling to describe functional properties were employed. Regression equations were developed to define staling-softness effects for the investigated emulsifiers. Synergistic responses are also identified. Potential commercial applications via computerization are discussed to assist in selecting emulsifier systems for specific functional applications.

INTRODUCTION

Automated continuous production processing in the bread industry has created in increased demand for emulsifier systems which demonstrate functional versatility in bread softening and dough conditioning. A variety of emulsifiers differing in type and physical form subsequently have been developed to meet this demand in an expansive bread emulsifier market. Those presently used must comply with the Federal Standards of Identity (1) for Bakery Products, which regulate their use by prescribing allowable types and usage levels. Many of them are categorized by their efficacy in producing bread softening and/or dough conditioning effects. Their value in providing the necessary performance is, therefore, well recognized by the bread industry.

The literature describes numerous investigations of the softening/conditioning properties of FDA regulated emulsifiers utilized in the manufacture of continuous mix bread (2-8). Very few authors have treated the experimental data statistically or developed mathematical models to establish data banks and compare functionality. Information often is presented in the form of raw data measurements, which must be analyzed to extract useful information. Model development forces a critical examination of existing data and yields a statement of their quantitative relationships. Modeling strategy permits optimization of emulsifier type and usage level, thereby improving production economics and product quality.

The application of mathematical modeling as an accurate and credible tool to predict and assess softening/conditioning properties of emulsifier systems in continuous mix bread will be reviewed. This method offers an alternative to the cumbersome practice of selecting an acceptable softener/conditioner system through extensive experimentation.

EXPERIMENTAL PROCEDURES

Continuous Mix Bread Process

The softener/conditioner systems were evaluated utilizing a laboratory model continuous dough mixing unit. The bread formulation is illustrated in Table I. Emulsifier systems were evaluated at 0.5% level by weight, basis flour. When both the softening and conditioning agent comprised the emulsifier system, each contributed 0.25% by weight to the total system. Preferments were set at 90 F for 2 hr. After this period, a "spike" consisting of sugar and all of the nonfat dry milk solids was introduced into the fermented brew. The brew temperature was reduced to 60-65 F before utilization. The softener/conditioner systems were diluted with soybean oil, placed into a heated fat tank, and metered at 3.0% by weight (emulsifier plus soybean oil) basis flour level into the pre-mix stage of the continuous mixing unit.

Developer speeds were set at either 132 or 138 revolutions per min (rpm) to produce a dough that was optimally developed. Dough temperature was maintained at 98-102 F. Dough was scaled at 15.5 oz into pans that were 3 in. high, 10 x 5 in. top measurement, and 9.25 x 4.25 in. bottom measurement. Doughs were proofed to 0.75 in. above the pan to produce an expanded loaf. Bread produced in this manner undergoes severe treatment in both scaling weight and subsequent proof height. Proofing time varied from 50 to 70 min, depending on the softener/conditioner system utilized. Six loaves were baked for 15 min at 460 F, cooled for 60 min, weighed, and their volume determined by the rapeseed displacement method. Three of the six loaves produced were shock tested.

Shock Loss Evaluation

Shock evaluation, which measures the effectiveness of the dough conditioner in the emulsifier system, was performed as follows. The panned, proofed loaves were allowed to roll down 3 ft of a 5 ft length of roller conveyor inclined at a 16.5° angle; then the loaves were stopped

TABLE I

Continuous Mix Bread Formula

Ingredient	Percent	
Bread flour	100.00	
Water	65.00	
Sugar	2.00	
Salt	2.00	
Sodium propionate	0.10	Brew
Yeast	3.25	
Yeast food	0.75	
Potassium bromate	60 ppm	
Potassium iodate	15 ppm	
Sugar	5.00	Spike
Nonfat dry milk solids	2.00	
Softener/conditioner	0.50	
Liquid soybean oil[a]	2.50	

[a]Contains 4% soybean stearine.

TABLE II

Experimental Design Schematic[a]

			Dough conditioning agent		
Bread softener	Soybean oil[b]	LEC (Lecithin)	HLEC (Hydroxylated lecithin)	SMG	EOM (Ethoxylated monodiglyceride)
Soybean oil[b]	1	2	3	4	5
MG (Monodiglycerides)	6	7	8	9	10
PGME (Propylene glycol monoester)	11	12	13	14	15
LEC (Lecithin)	–	–	16	17	18
SMG (Succinylated monodiglycerides)	–	–	19	–	20
SSL (Sodium stearoyl-2-lactylated)	21	22	23	24	25
CSL (Calcium stearoyl-2-lactylate)	26	27	28	29	30
LS (Lactylic stearate)	31	32	33	34	35

[a]Integer in design identifies softener/conditioner system.
[b]Contains 4% soybean stearine.

abruptly by a permanently affixed metal stop at the end of the conveyor. This test is described by another investigator (9) and represents a severe simulation test of the conditions to which a proofed loaf may be exposed during transfer from proofer to oven in a commercial operation. Volume differences between shocked and unshocked loaves were calculated and compared.

Calculation:

$$\% \text{ Shock Loss} = \frac{\text{Specific Volume Lost by Shocking} \times 100}{\text{Unshocked Specific Volume}}$$

Bread Softeness Measurement

The bread softness retention properties were measured over a 7-day storage period. The softening effect is measured by an Instron rheological instrument. This instrument measures the amount of work required to compress the crumb of a loaf of bread. The measurement is recorded in inch-grams (a unit of work or energy required to move 1 gram a distance of 1 inch).

Linear regression analysis is performed on the collected data for bread softness retention properties. The literature is replete with articles on the subject of linear regression. The regression coefficients are determined using Gauss' principle of least squares (10-12). Not knowing the theoretical functional equation, one employs a linear function of the casual independent variable, called a predictor, to explain the effect of the system on the dependent response variable. The linear regression equation assumed to describe the system is:

(1) $Y = \beta_0 + \beta_1 E_1$ where
Y = Response
β_0 = Intercept
β_1 = Slope (Bread Softness Rate of Change)
E_1 = Independent Variable or Time

Mathematical Models

This investigation utilized the interaction model equation, assuming the softener and conditioner would demonstrate a synergistic relationship. The equation characterizing the model for response Y takes the form of:

$$(2)\ Y = \beta_{S_i} (\% S_i) + \beta_{C_j} (\% C_j) + \beta_{S_i C_j} (\% S_i)(\% C_j)$$

where S_i = softener, C_j = conditioner.

The β coefficients in the model are determined algebraically by solving for three unknowns in three equations. A Fortran computer program was employed to determine these coefficients.

Binary Mixture Experimentation

The softener/conditioner systems were investigated in the binary mixture design shown in Table II. The numbers identify the emulsifier combination, e.g., No. 18 consists of lecithin and ethoxylated monodiglycerides. The experimentation was randomized and did not follow the order as shown in Table II.

Each emulsifier in the vertical column (softener) was evaluated in combination with each dough conditioner in the horizontal row. Two emulsifiers (lecithin and succinylated monodiglycerides) were evaluated as both a softener and conditioner. When both the softener and conditioner were combined to form a complete system, each contributed equally (0.25%) by weight to the total system. Each emulsifier was also individually investigated for the various functional responses at the 0.5% level. This was required to establish a basis for determining possible emulsifier interaction or synergism with the complementary component in a softener/conditioner system.

RESULTS AND DISCUSSION

Functional data consisting of bread softness retention, shock loss tolerance, and bread volume served as the basis for developing Figure 1, which indicates the relative position (rank) of an emulsifier system in relation to the remaining field. This is an exhibition which illustrates the composite functional characteristics for the investigated emulsifier systems. The data in this figure are based on a single experimentation. A Fortran computer program was utilized to sort the response data and functionally rank the systems. Systems ranking first in shock loss tolerance, bread softness retention, and bread volume are respectively: LS-EOM (No. 35), LS (No. 31), and CSL (No. 26). The least functional systems for the preceding respective categories are MG (No. 6), MG/HLEC (No. 8), and SMG/HLEC (No. 19).

Theoretical values or coefficients were assigned for the functional properties deemed most important by continuous mix bread manufacturers. Overall Performances Indices (PI) were computed to determine a composite functionality index.

Softness retention and shock loss tolerance are each assigned an importance value or coefficient of 40. Bread volume was rated at 20. Utilizing data in Figure 1 as a source for emulsifier percentile rank, one employs the following expression to compute Performance Indices for the investigated emulsifier systems.

$$(3)\ \text{Performance Indes (PI)}_i = 40\ (\text{Softness Retention \% Rank}) + 40\ (\text{Shock Loss Tolerance \% Rank}) + 20\ (\text{Bread Volume \% Rank})$$

for i = 1 to 35 (See Table II)

The highest theoretical Performance Index would be 100. The following example illustrates the PI calculation for softener/conditioner system No. 31.

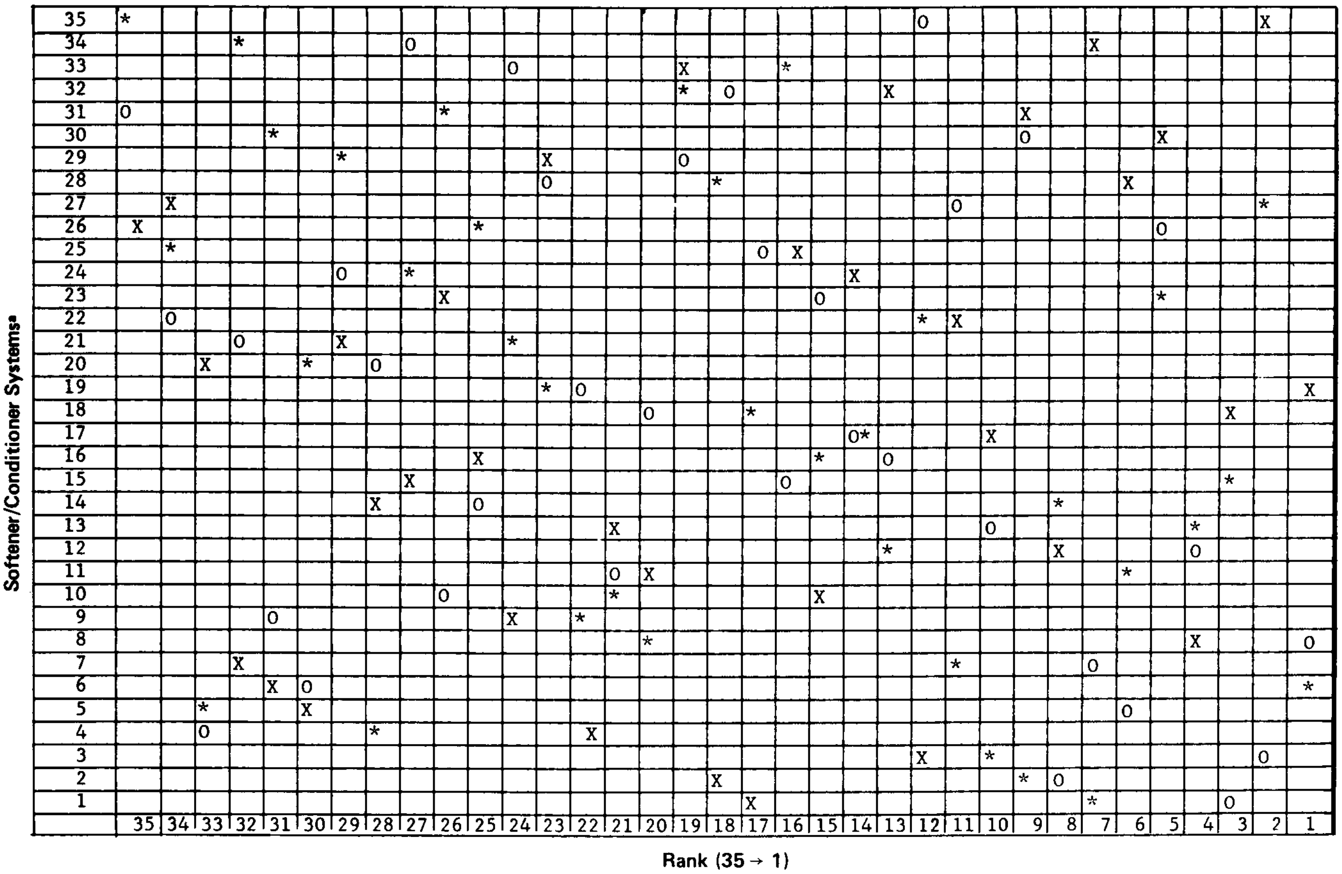

FIG. 1. Functional response rank for softener, conditioner, and softener/conditioner systems (Rank 1 is lowest). * = Shock loss tolerance; O = softness retention; X = bread specific volumes. [a]See Table II.

$$\text{Softness retention percentile rank} = \frac{35}{35} = 1.0$$

$$\text{Shock Loss Tolerance Percentile Rank} = \frac{26}{35} = 0.74$$

$$\text{Bread Volume Percentile Rank} = \frac{9}{35} = 0.26$$

$$(\text{Performance Index})_{31} = 40\,(1.0) + 40\,(0.74) + 20\,(0.26) = 75$$

Figure 2 shows a bar diagram indicating PIs for all the investigated emulsifiers and emulsifier combinations. Systems possessing indices of 75 or higher are: LS, SMG, MG/SMG, SSL, and SMG/EOM.

The functional characteristics initially are analyzed through graphical representations of conditioner/softener interaction responses. Figure 3 illustrates the interaction effects of dough conditioners lecithin (C_1), hydroxylated lecithin (C_2), SMG (C_3), and EOM (C_4) with the softeners (S_i) on bread crumb firming rate. The softener/conditioner response point is located on the vertical broker (---) axis line in each quadrant. The curves which connect the three points that exhibit a "concave up" contour indicate a negative softener/conditioner interaction (synergism) for the specified functional response. A "concave down" configuration implies that a positive interaction (synergism) has occurred. Positive or negative synergism can also be determined by sketching a straight line from the conditioner response data point to the softener response point as shown in Figure 3, between C_1 and S_5. When a proportionally additive effect on firming rate is presumed, the straight line should intersect the broken (---) vertical axis line at the C_1/S_5 combination measured response point. However, in this situation, the measured response point does not agree with the proportionally additive point. An interaction (synergism) between the emulsifiers C_1 and S_5 is observed by noting the distance difference between X_5 and the point

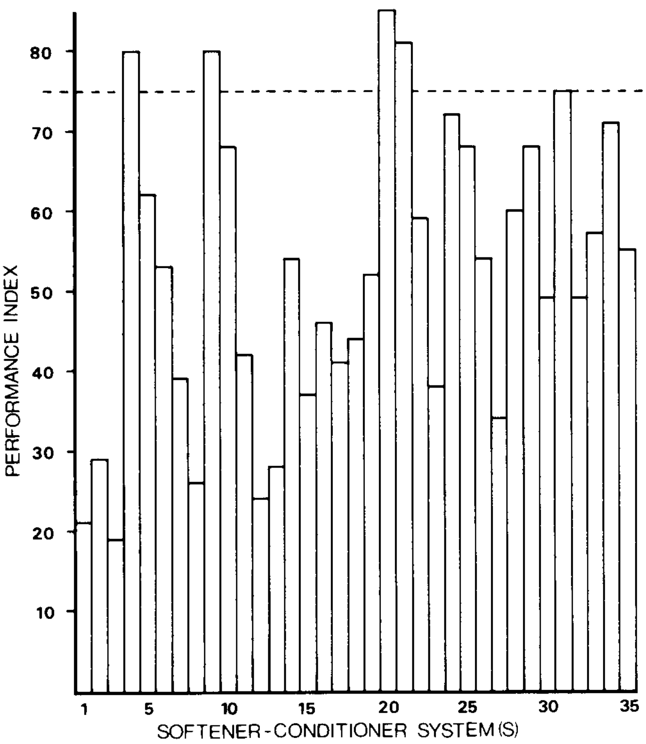

FIG. 2. Calculated performance indices (PI) for softener/conditioner systems.

where the straight line connecting the points C_1 and S_5 bisects the vertical response axis. Response points falling above the straight line between C_1 and S_5 are indicative of negative interactions. A positive interaction or synergism

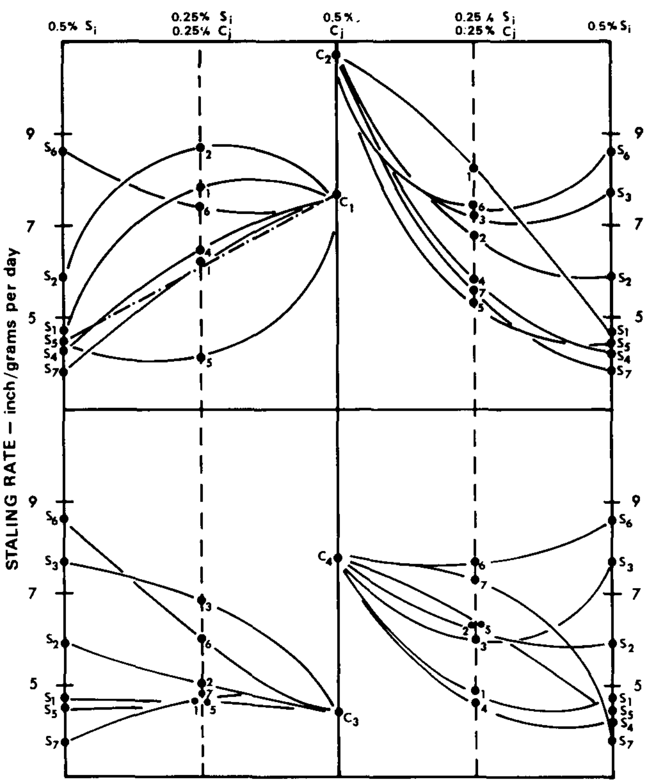

FIG. 3. Graphical representations for softener $(S_i)^a$ - conditioner $(C_j)^b$ effect on bread crumb firming rate. (a) S_1 Mono-Di, S_2 PGME, S_3 Lecithin, S_4 SMG, S_5 SSL, S_6 CSL, S_7 LS; (b) C_1 Lecithin, C_2 Hydroxylated lecithin, C_3 SMG, C_4 EOM. Abbreviations: PGME = propylene glycol monoester, SMG = succinylated monodiglycerides, SSL = sodium stearoyl-2-lactylate, CSL = calcium stearoyl-2-lactylate, LS = lactylic stearate, EOM = ethoxylated monodiglyceride.

indicates increased functionality.

Graphical representations for the remaining emulsifier responses of shock loss and bread volume are shown in Figures 4 and 5. The same method of interpretation as in the preceding discussion can be applied to these figures.

Mathematical models describing softener/conditioner functionality based on criteria of bread softness retention, shock loss, and bread specific volume are presented. Coefficients for the model equations in each functional category are exhibited in Table III.

An example illustrating the utilization of this information to describe the functional properties of a given softener/conditioner follows. With system 12, selected arbitrarily, as the subject of our example, the coefficients (A_1,A_2,A_3) for the models are taken from Table III and inserted into the equations. The following equations describe system 12 (PGME-lecithin);

$$\text{Bread Volume} = Y = 12.78\ C_j + 12.82\ S_i - 1.60\ C_j\ S_i$$
$$\text{Shock Loss} = Y = 63.8\ C_j + 65.8\ S_i - 30.4\ C_j\ S_i$$
$$\text{Bread Softness Retention} = Y = 15.49\ C_j + 11.94\ S_i + 30.35\ C_j\ S_i$$

The sign on coefficient A_3 indicates whether the interaction/synergism is positive (+) or negative (-).

The terms C_j and S_i are expressed in percent (decimal) when applying these equations. These equations have applications not only as predictive tools to estimate a certain quantitative functional response, but also to estimate the composition for a softener/conditioner system which yields an acceptable performance level. For example, assume a commercial operation is employing a softener/conditioner system composed of PGME/EOM. For inventory reasons, the PGME component is no longer available.

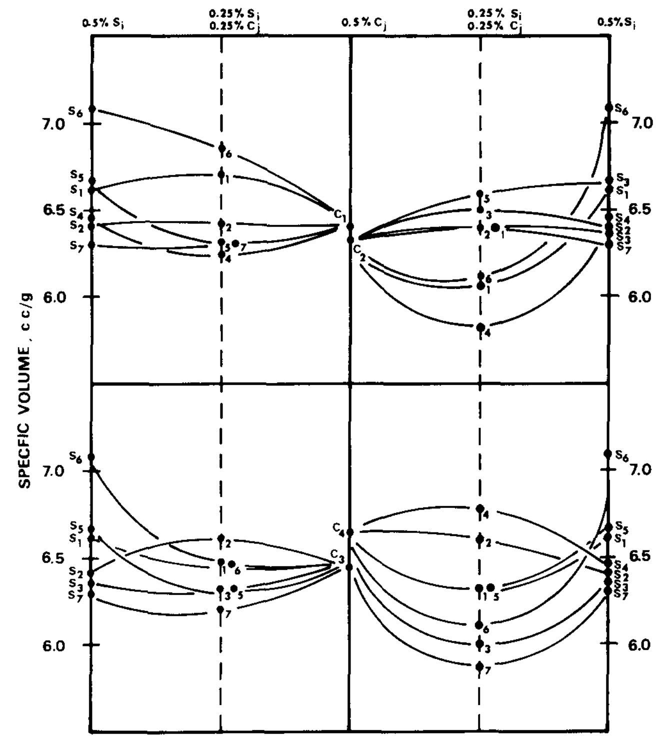

FIG. 4. Graphical representations for softener $(S_i)^a$ - conditoner $(C_j)^b$ effect on bread volume. (a) S_1 Mono-Di, S_2 PGME, S_3 Lecithin, S_4 SMG, S_5 SSL, S_6 CSL, S_7 LS; (b) C_1 Lecithin, C_2 Hydroxylated lecithin, C_3 SMG, C_4 EOM. Abbreviations: PGME = propylene glycol monoester, SMG = succinylated monodiglycerides, SSL = sodium stearoyl-2-lactylate, CSL = calcium stearoyl-2-lactylate, LS = lactylic stearate, EOM = ethoxylated monodiglyceride.

However, the supply of SMG in his warehouse is substantial. Assuming quality assurance requires a 6.4 cc/g bread specific volume, one asks how much SMG is required to meet this quality standard for volume. Utilizing the model equation describing the SMG/EOM system for bread volume and the EOM level at 0.25%, operations on the following equations to solve for S_i follow:

$$Y = 13.28\ C_j + 12.90\ S_i + 3.44\ C_j\ S_i$$
$$Y = 6.4\ cc/g = 13.28\ C_j + 12.90\ S_i + 3.44\ C_j\ S_i$$
$$6.4 - 13.28\ C_j = 12.90\ S_i + 3.44\ C_j\ S_i$$
$$6.4 - 13.28\ C_j = S_i\ (12.90 + 3.44\ C_j)$$
$$\frac{6.4 - 13.28\ C_j}{12.90 + 3.44\ C_j} = S_i$$
$$\frac{6.4 - 13.28\ (0.25)}{12.9 + 3.44\ (0.25)} = S_i$$
$$0.224 = S_i$$

Based on the above calculations, a similar bread volume response of 6.4 cc/g can be obtained with 0.22% SMG and 0.25% EOM where it previously necessitated 0.25% PGME and 0.25% EOM. The preceding example is one of many potential applications for the model equations.

A flow diagram shown in Figure 6 illustrates on a computer basis a hypothetical operation utilizing models for selection and optimization of bread emulsifiers in a commercial bakery. Emulsifier experimentation is initially required to generate functional data for the development of mathematical models. This basic information is subsequently stored in a data bank identifying the functional properties of the emulsifiers and/or emulsifier combinations in that specific plant operation. Input regarding emulsifier inventory and economics, quality assurance functional

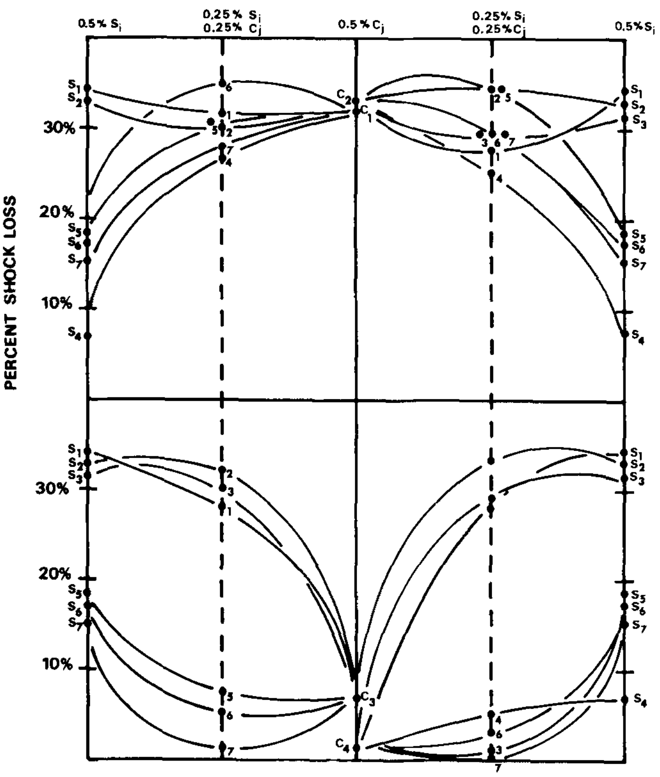

FIG. 5. Graphical representations for softener $(S_i)^a$ - conditioner $(C_j)^b$ effect on percent shock loss. (a) S_1 Mono-Di, S_2 PGME, S_3 Lecithin, S_4 SMG, S_5 SSL, S_6 CSL, S_7LS; (b) C_1 Lecithin, C_2 Hydroxylated lecithin, C_3 SMG, C_4 EOM. Abbreviations: PGME = propylene glycol monoester, SMG = succinylated monodiglycerides, SSL = sodium stearoyl-2-lactylate, CSL = calcium stearoyl-2-lactylate, LS = lactylic stearate, EOM = ethoxylated monodiglyceride.

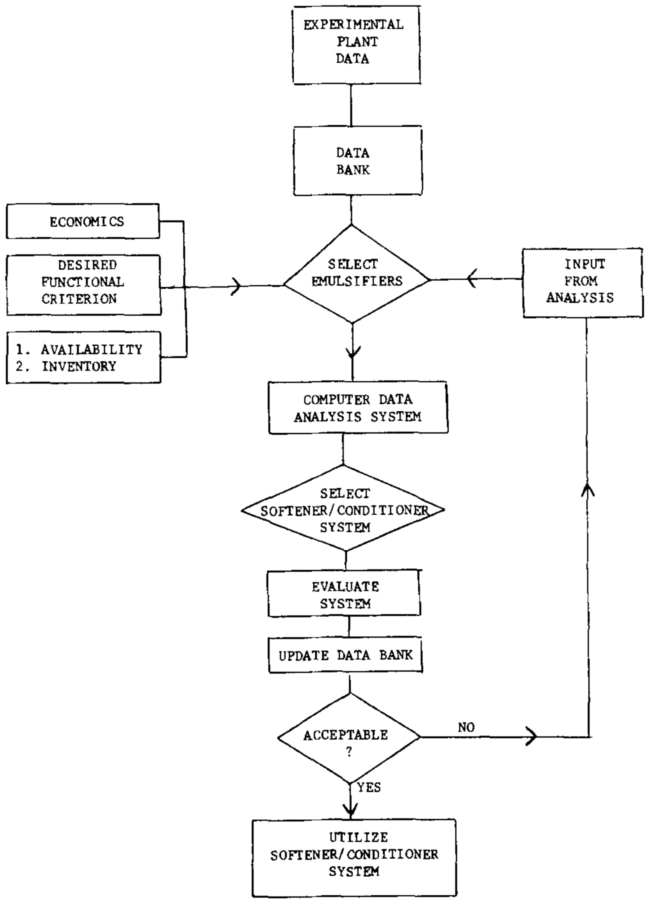

FIG. 6. Flow chart for commercial application–selection of bread emulsifier systems via computerization.

TABLE III

Coefficients for Model Equations Characterizing Functional Properties of Softener/Conditioner Systems and Subsequent Emulsifier Interaction

Model: $Y = A_1 * (\% C_j) + A_2 * (\% S_i) + A_3 * (\% C_j)(S_i)$

	Bread volume			Shock loss			Staling rate		
System number[a]	A_1	A_2	A_3	A_1	A_2	A_3	A_1	A_2	A_3
7	12.78	13.28	2.96	63.8	69.2	−23.2	15.49	9.47	24.97
8	12.66	13.28	−6.64	63.6	69.2	−78.4	21.43	9.47	−63.6
9	12.9	13.28	−1.04	14.0	69.2	116.8	8.8	9.47	2.14
10	13.28	13.28	−4.80	2.8	69.2	161.6	15.77	9.47	−23.33
12	12.78	12.82	−1.60	63.8	65.8	−30.4	15.49	11.94	30.35
13	12.66	12.82	0.96	63.6	65.8	24.8	21.43	11.94	−12.5
14	12.90	12.82	2.88	14.0	65.8	200.8	8.80	11.94	−2.88
15	13.28	12.82	1.20	2.8	65.8	268.0	15.77	11.94	−11.78
16	12.66	12.78	2.08	63.6	63.8	−31.2	21.43	15.49	−32.22
17	12.90	12.78	−1.60	14.0	63.8	168.8	8.8	15.49	11.23
18	13.28	12.78	−8.08	2.8	63.8	202.4	15.77	15.49	−28.57
19	12.66	12.90	−9.28	63.6	14.0	91.2	21.43	8.80	−28.25
20	13.28	12.90	3.44	2.8	14.0	12.8	15.77	8.80	−22.26
22	12.78	13.26	−3.04	63.8	37.2	92.0	15.49	9.09	−32.71
23	12.66	13.26	1.76	63.6	37.2	137.6	21.43	9.09	−21.97
24	12.90	13.26	−3.36	14.0	37.2	−84.8	8.8	9.09	4.23
25	13.28	13.26	−4.56	2.8	37.2	−152.0	15.77	9.09	−0.83
27	12.78	14.34	1.12	63.8	35.2	151.2	15.49	17.36	−12.14
28	12.66	14.34	−9.12	63.6	35.2	73.6	21.43	17.36	−63.9
29	12.90	14.34	−5.60	14.0	35.2	−107.2	8.80	17.36	−8.12
30	13.28	14.34	−12.56	2.8	35.2	−102.4	15.77	17.36	−9.07
32	12.78	12.6	−0.24	63.8	30.4	84.0	15.49	7.74	5.6
33	12.66	12.6	1.36	63.6	30.4	94.4	21.43	7.74	−25.7
34	12.90	12.6	−2.80	14.0	30.4	−148.8	8.80	7.74	10.37
35	13.28	12.6	−9.60	2.8	30.4	−132.8	15.77	7.74	21.99

[a]See Table I for exact emulsifier composition.

criteria, and other applicable information is then incorporated into the program. An instruction to determine all possible softener/conditioner systems meeting the given constraints, channels the program into the data analysis system. From this analysis, emulsifier systems meeting the required functionality are identified. Emulsifier systems meeting the stipulated composite functionality are then experimentally evaluated (in bread) to determine bread production applicability. Results of this evaluation are then transmitted to the data bank for future reference. This action is necessary even though the system does or does not meet the functional criteria. The predicted functionality responses can be compared with the empirical data, thereby allowing a correction factor to be incorporated into the original model equation. The operation is complete if the designated softener/conditioner system is functionally acceptable. If not, the procedure can be repeated utilizing the modified model and the same emulsifier system or selecting another emulsifier combination. Factors affecting the functional responses such as variability in flour (protein content), miscellaneous bread ingredients, plant conditions, etc., would have to be integrated into the computer system to fully optimize the entire operation for efficiency and accuracy.

This study demonstrates a scientific and systematic approach in developing comparative functional data and establishing functional relationships between various emulsifiers in formulating softener/conditioner systems for continuous mix bread manufacture. Utilization of modeling techniques provides a more accurate tool to assess and chracterize emulsifier functionality, thereby reducing optimization efforts when commercially applied.

ACKNOWLEDGMENTS

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