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Model for Predicting the pH of Foods Comprising Mixtures of Tomatoes and Low-Acid Ingredients

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ABSTRACT

The possibility of predicting the pH of home-canned foods comprising mixtures of tomatoes and low-acid ingredients was investigated. A quadratic model representing multi-component mixtures of tomatoes and nine low-acid ingredients, combined in various proportions, was tested. A 19-term equation for pH prediction, generated from the data, yielded a correlation coefficient of 0.9998 and a standard error of 0.11 pH unit. Tomato acidity was an important determinant of product pH. The equation was validated by comparing the predicted and observed pH of 55 representative products. Good agreement between these pH values was obtained. Criteria for recognition of low-acid products were established.

The pH of food products comprising combinations of low-acid and high-acid ingredients, such as tomato juice cocktail, stewed tomatoes and spaghetti sauce, may be above or below 4.6, depending on the ingredient proportions specified by their recipes (*11*). If these "combination foods" are to be home-canned, their pH becomes a critical factor in process selection since low-acid foods (pH >4.6) must be pressure-canned to destroy spores of *Clostridium botulinum* while high acid-foods (pH ≤4.6) may be processed in a boiling water bath (*1,8*). Published guidelines for home-canning of combination foods generally call for use of a process appropriate to the highest pH (least acidic) ingredient (*2,8*) or to the low-acid ingredient requiring the longest processing time when processed alone (*7*). We have noted many deviations from these guidelines in the home canning literature (*3,11*), a situation at best likely to confuse home canners, and in some instances, to result in the gross underprocessing of low-acid foods (*4,5*), thereby increasing the risk of botulism. Extension specialists and other publishers of home-canning information need better guidelines to distinguish between low-acid and high-acid combination foods so that appropriate processing recommendations can be made.

In a previous study of potential criteria for process selection, we determined the pH limits of a number of important categories of tomato-based combinations, based on the analysis of representative products (*11*). Our objective in the present study was to develop the capability of predicting the pH of specific tomato-based combination foods from recipe data by means of regression equations derived from a model simulating such combinations. This capability would enable extension specialists to screen old or new home canning recipes to determine the suitability of the specified processing method and, if necessary, to recommend safer processes.

MATERIALS AND METHODS

Design of model

Based on results of exploratory studies, we developed an experimental design for a quadratic model representing mixtures of tomatoes and low-acid ingredients. Data on product composition, taken from our compilation of recipes for combination foods (*11*), were used to select the low-acid ingredients most frequently used in important categories of combination foods. The design consisted of a number of statistically balanced trials, each representing different ingredient combinations, similar to that described by Hare (*6*). Low-acid ingredients included green bell peppers, mushrooms, carrots, red kidney beans, chopped onions, celery, chicken broth, beef broth and ground beef. The following trials were tested in this study: (*a*) single ingredients - 5 to 15 trials, each trial corresponding to a portion taken from every new package used in the study so that ingredient variability could be determined; (*b*) two-way combinations - mixtures of each ingredient with 20, 40, 60 and 80% tomatoes (36 trials); (*c*) three-way combinations - mixtures of 20, 40, 60 and 80% tomatoes with equal parts of two other ingredients, e.g., 40% tomatoes with 30% carrots and 30% onions (144 trials) and (*d*) multicomponent combinations - mixtures of 20% tomatoes with 48% of one other component and 4% of each remaining ingredient (9 trials); 40% tomatoes with 33-34% of one other component and 3-4% of each remaining ingredient (9 trials); 60% tomatoes with 24% of one other component and 2% of each remaining ingredient (9 trials); and 80% tomatoes with 12% of one other component and 1% of each remaining ingredient (9 trials); and mixtures of 20%, 40%, 60%, and 80% tomatoes with equal parts of each of the nine other ingredients (4 trials).

Because of the critical role of tomatoes as the only high-acid ingredient in the model, these trials were carried out with four different tomato varieties. In 1979, a typical home garden hybrid tomato, Burpee

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TABLE 2. *Regression coefficients and statistics for prediction of mixture pH.*

Parameter	Ingredient	Regression coeff.	Standard error (x 10^4)	Sum of squares
β_0	Tomato	0.0446	1.09	9124
β_1	Ground beef	0.0633	2.81	1087
β_2	Mushroom	0.0596	2.81	914
β_3	Onion	0.0486	3.70	481
β_4	Green bell pepper	0.0494	2.73	662
β_5	Celery	0.0552	3.37	583
β_6	Beef broth	0.0589	2.73	815
β_7	Carrot	0.0498	2.81	580
β_8	Chicken broth	0.0623	2.73	865
β_9	Kidney bean	0.0587	2.52	907
β_{01}	Tomato-ground beef	-0.00011	0.13	0.9
β_{02}	Tomato-mushroom	-0.00020	0.13	2.9
β_{03}	Tomato-onion	-0.00005	0.14	0.1
β_{04}	Tomato-green bell pepper	-0.00006	0.13	0.3
β_{05}	Tomato-celery	-0.00016	0.14	1.6
β_{06}	Tomato-beef broth	-0.00025	0.13	4.5
β_{07}	Tomato-carrot	-0.00008	0.13	0.5
β_{08}	Tomato-chicken broth	-0.00025	0.13	4.9
β_{09}	Tomato-kidney bean	-0.00003	0.13	0.1

the coefficient. As can be seen from the sum of squares values, the combination terms were of far less importance than the individual ingredient terms. Tomato, the primary source of acidity in these mixtures, had the greatest effect on the regression, based on the sums of squares. Among the low acid components studied, ground beef, mushroom, kidney bean and the broths exerted the greatest effect on the regression.

Validation of model

The validity of the model for pH prediction (19-term regression equation, pooled 1979 data) was tested by comparing predicted and actual pH values for representative combination products prepared in our laboratory (Fig. 1). These samples included two tomato juice blends, seven tomato soups, seven mixed vegetable dishes, 27 meatless tomato sauces, four tomato-meat sauces and three chili products. Differences between the observed and predicted pH values showed no consistent direction and were not significantly different from zero at the 5% level (t = 0.31). The mean difference (absolute value) between the observed and predicted pH values was 0.12 pH unit. Ninety percent of the predicted pH values were within two standard errors (0.22 pH unit) of the observed pH values. Most of the larger discrepancies between predicted and observed pH values occurred with higher pH products.

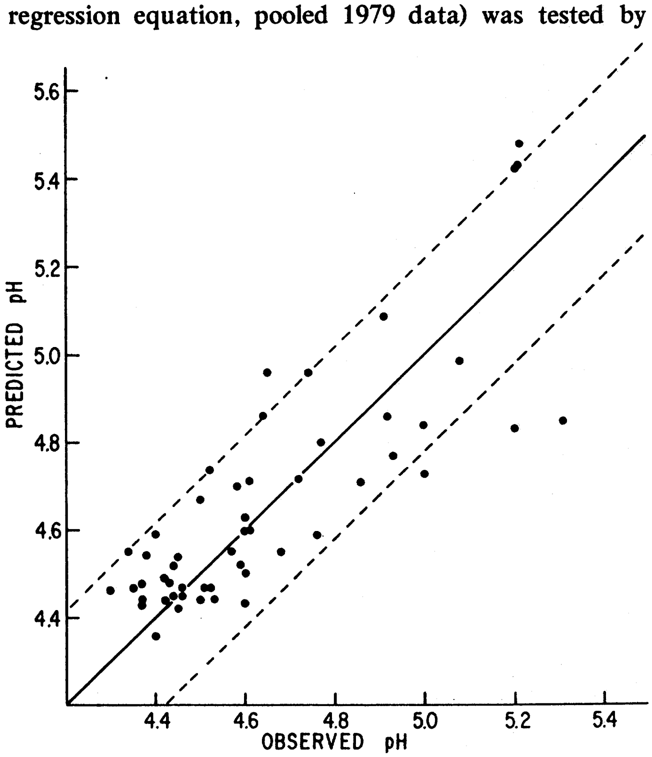

Figure 1. *Predicted and observed pH values of representative tomato-based combination foods.*

Effect of tomato acidity on pH prediction

The dispersion of points in Fig. 1 may have been in part due to variation in the acidity of tomatoes used to prepare the combination foods being tested. To demonstrate the effect of tomato acidity on prediction of mixture pH, we generated regression equations from data acquired with three tomato varieties: Ace 55 VF, Roma VF, and Rutgers, having mean pH values of 4.58, 4.45, and 4.34, respectively.

The primary effect of tomato acidity on the regression equations was an increase in the tomato regression coefficient β_0 with increasing tomato pH (Table 3). Changes in the other regression coefficients were small and not indicative of any trends. We have examined the extent to which tomato acidity affects the prediction of pH by recalculating the pH of the 50 products tested previously, employing the new regression equations. The absolute value of differences between predicted and observed pH values was not greatly affected by the choice of equation. However, predictions based on Ace 55 VF

VF hybrid, and a typical pear-shaped paste-type tomato, Roma VF, were used. An abbreviated version of the model (no three-way combinations) was tested in 1980 with three tomato varieties known to differ in pH (9): Ace 55 VF, Roma VF and Rutgers.

Ingredients for trials

All tomato samples were obtained from Fordhook Farms in Doylestown, PA. The tomatoes were canned without added salt or acidulant in a boiling water bath by the USDA raw pack home canning process (1). Green bell peppers of the Yolo Wonder L variety also were obtained from Fordhook Farms. The peppers were packed with added boiling water, but no salt or acidulants, and pressure canned at 10 psi according to the Ball Blue Book process (2). Commercially canned mushrooms (stems and pieces), carrots, red kidney beans, chicken broth, beef broth and frozen chopped onions and ground beef patties were purchased in case lots from local supermarkets. Celery was purchased fresh, as required. Frozen ingredients were stored at -18°C; all other ingredients were refrigerated at 5°C until needed.

Preparation and analysis of combinations

All ingredients were combined at room-temperature. The canned green peppers, mushrooms, carrots and red kidney beans were drained before being used. The raw ingredients (ground beef, chopped onions, celery) were thawed if necessary, steam-blanched for 2 min at 100°C, and then air-cooled to room temperature. Individual ingredients were pureed for 30 sec at high speed in a Waring Blendor. Mixtures and single ingredient samples corresponding to each trial were prepared in 100-g quantities from the pureed ingredients, thoroughly mixed and the pH was determined.

Statistical analysis

The statistical analysis of the data collected in these trials was performed for each tomato variety separately, and also for the combined data set for Roma VF and Burpee VF hybrid tomatoes (1979 trials). Regression equations for predicting pH were obtained by fitting the data to the model:

$$(1)\ \ pH = \sum_{i=0}^{9} \beta_i X_i + \sum_{i<j=1}^{9} \beta_{ij} X_i X_j$$

where β_i is the regression coefficient and X_i, the ingredient percentage (by weight) for ingredient i, respectively; where β_{ij} is the regression coefficient for the combination of ingredient i and j; and where i and j assume the following values ($j \neq 0$):

0 - tomatoes	5 - celery
1 - meat	6 - beef broth
2 - mushrooms	7 - carrots
3 - onions	8 - chicken broth
4 - peppers	9 - beans

The initial results showed that most terms $\beta_{ij}X_iX_j$ ($0 < i < j \leqslant 9$) were not important in that the β_{ij} values were not significantly different from zero. The model was then simplified from 55 to 19 terms:

$$(2)\ \ pH = \sum_{i=0}^{9} \beta_i X_i + \sum_{j=i}^{9} \beta_{0j} X_0 X_j$$

In other words, only those terms representing each individual ingredient and the products of these percentages with the percentage of tomato in the mixture were considered.

We tested the simplified equations by comparing calculated and experimentally determined pH values for 50 products representing important categories of combination foods that we had prepared, canned and analyzed previously for another investigation (11). We also tested the equations with 26 additional combination foods prepared with tomatoes for which we had pH data. The significance of the difference between the observed and predicted pH values was determined with the Student's t distribution.

RESULTS

Regression equations for prediction of mixture pH

Statistics for prediction of mixture pH by the exact (55-term) and simplified (19-term) regression equations with Burpee VF hybrid and Roma VF tomatoes are given in Table 1. These results show that the simplified equation could be used instead of the more cumbersome exact equation without significantly affecting the correlation coefficient or standard error of the estimate. Similarly, the data acquired with Burpee VF hybrid and Roma VF tomatoes, which had similar pH values (4.39 and 4.36, respectively), could be pooled to give a single regression equation.

Regression coefficients corresponding to each individual ingredient and to combinations of each low acid ingredient with tomatoes (19-term equation, 1979 pooled data) are given in Table 2. Also shown for each regression coefficient are values of the standard error and the sum of squares, an indication of the relative importance of each term in the equation. The 95% confidence limits (two standard errors) of the regression coefficients for individual ingredient terms represented no more than 1.5% of the value of the coefficient; the 95% confidence limits for the low-acid ingredient-tomato combination terms varied from 5 to 43% of the value of

TABLE 1. *Comparison of statistics for pH prediction by 55-and 19-term regression equations with Burpee VF hybrid and Roma VF tomatoes (1979 data).*

Tomato variety	No. trials	No. terms in equation	Correlation coeff.	Stand. error of estimate
Burpee VF hybrid	323	55	0.9998	0.10
		19	0.9997	0.11
Roma VF	334	55	0.9998	0.10
		19	0.9997	0.12
Pooled	657	19	0.9997	0.11

TABLE 3. *Effect of tomato pH on regression equations for prediction of mixture pH.*

Data set for regression	Mean tomato pH	Regression coeff. βo	Predicted vs observed pH	
			Mean difference[a]	Bias[b]
Ace 55 VF	4.58	0.0464	0.16	Positive[c]
Roma VF	4.45	0.0448	0.13	0
Rutgers	4.34	0.0438	0.13	Negative[c]
Pooled (1979)	4.36/4.39	0.0446	0.12	0

[a]Absolute value.
[b]Predicted-observed pH.
[c]Difference between predicted and observed pH significantly different from zero at 0.01 level.

TABLE 4. *Effect of high acid and low acid tomatoes on observed and predicted pH of combinations.*

Product	Recipe no.	Observed pH		Predicted pH		
		Tomato	Product	Rutgers equation	1979 Equation	Ace 55 VF equation
Tomato sauce	378	4.26	4.36	4.35	4.47	4.57
Marinara sauce	226	4.25	4.40	4.39	4.50	4.66
Tomato sauce	077	4.32	4.36	4.35	4.45	4.61
Tomato sauce	230	4.53	4.62	4.34	4.47	4.56
Marinara sauce	295	4.57	4.59	4.39	4.49	4.66
Tomato sauce	076	4.51	4.55	4.35	4.45	4.61

tomatoes were consistently high (positive bias), while predictions based on Rutgers tomatoes were consistently low (negative bias).

These biases are indicative of the observed pH of combination foods prepared with high- or low-acid tomatoes. We measured both the tomato pH and the product pH for 26 tomato-based combination foods selected to test the new regression equations. The pH data for those products prepared with the most acidic and the least acidic tomatoes are given together with pH predictions based on the Rutgers, pooled 1979 data, and Ace 55 VF regression equations in Table 4. These results clearly show the greater accuracy of the Rutgers equation with products prepared with low pH tomatoes and of the Ace 55 VF equation with products prepared from high pH tomatoes.

DISCUSSION

The regression equations for pH prediction described herein might be used by extension specialists or other professionals knowledgeable in home food preservation to determine whether the method of processing specified by a home-canning recipe for a tomato-based combination food product is consistent with the product's pH. This capability would be useful for screening old or new recipes published by the media, by manufacturers of home-canning equipment, or by government agencies or recipes submitted by private individuals seeking advice. The regression equations cannot be used to determine the adequacy of specific processing times and temperatures. The equations are applicable to a wide variety of tomato-based combinations, including approximately half of the 400 recipes in our data bank (*11*).

The usefulness of the pH prediction depends on its accuracy, a reflection of the extent to which the model represents the food products being tested. The accuracy of pH predictions made with the 19-term regression equation (pooled 1979 data), as indicated by the magnitude and direction of differences between predicted and observed pH values, did not appear to be related to the product category. However, with products having very high pH values, i.e., greater than 4.8, the pH prediction was less accurate than with lower pH combinations. Differences between predicted and observed pH values for some high pH products may have resulted from the use of tomato ingredients (canned tomatoes, catsup) containing added acidulants, from the removal of meat and other low-acid ingredients from the final product by straining, from variations in the leanness of meat ingredients, and from other variations in the composition of fresh or processed ingredients.

In this study, the standard error of the regression for each of the data sets tested was approximately 0.1 pH unit. Therefore, a pH prediction could be made with 95% confidence within the limits of ±0.2 pH unit. If the 95% confidence limits for a prediction included a pH value greater than 4.6, that is, if the predicted pH exceeded 4.4, we would consider the combination as being a potential low-acid food. If this guideline were applied to the 76 pH predictions tested in our study, we would have correctly identified all of the 21 recipes that produced low acid products. We also would have identified an additional 12 recipes yielding borderline high-acid products (pH 4.55-4.60). We recommend that all untested home-canning recipes for tomato-based combinations, for which the predicted pH is between 4.4 and 4.6, be tested to confirm that they are, in fact, high-acid products (pH ≤4.6).

We have shown that combinations prepared with less acidic tomatoes are higher in pH than would be predicted by regression equations based on more typical tomatoes. These results point to a potentially hazardous situation that might arise if a home canner used a low-acid tomato variety like Ace 55 VF (*9,10*) or over-ripe tomatoes having a high pH (*10*) to prepare a combination product, following a published recipe originally tested with high acid tomatoes. The recipe probably would specify a boiling water bath process. Yet the product might have a pH exceeding 4.6, making the water bath process inadequate. This scenario, which could occur with 20 of 76 combination product recipes tested in our laboratory, could be avoided by (*a*) advising home canners to avoid using over-ripe tomatoes or specified varieties known to be high in pH as ingredients in combination products, and (*b*) advising home-canning specialists to avoid using atypically high-acid tomatoes in developing or testing home-canning recipes intended for publication.

CONCLUSIONS

A quadratic model for predicting the equilibrium pH of home-canned food products comprising mixtures of tomatoes and commonly used low-acid ingredients was developed. Regression equations derived from the model were applied to a wide variety of products and yielded unbiased predictions with a standard error of 0.1 pH unit. Tomato acidity was shown to be an important determinant of product pH. Criteria for recognition of low acid products were established, based on the 95% confidence limits of the prediction. Additional research is needed to determine the limitations of the model and adapt it for use by extension specialists in home food preservation.

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