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Effect of Fat Content on Flavor Delivery during Consumption: an in Vivo Model

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Data from studies of the effect of fat on in vivo flavor release were modeled to generate a predictive model (R^2 = 0.71). The data included a range of values from the literature and 200 new data points giving a total data set of 345 values; of these, 310 values were used as a data set for model development, and the remaining 35 values were used as a test set for model validation. The model could be used to estimate the differences in flavor delivery for samples with two different fat contents. The hydrophobicity of the flavor compounds was represented in the model by including log *P*. The model may provide a tool to aid in flavor reformulation between samples with different fat contents. Sensory analysis showed that an orange flavor present in a high-fat food could be reformulated for a low-fat food, giving a more similar flavor experience than in the absence of any formulation changes.

KEYWORDS: APCI-MS; flavor; aroma; lipid

INTRODUCTION

Fat has a significant effect on flavor partitioning and solubility in food products (*1*, *2*). However, flavor molecules are not locked away in fat droplets, but display a high level of mobility between the fat, aqueous phases, and headspace, allowing their release (*3*). Buttery et al. (*1*) described and modeled the effect of the oil fraction and oil/water partition coefficient on the partitioning of flavor in a static headspace situation. For lipophilic compounds the presence of fat can substantially decrease their headspace concentration, as the air/product partition coefficient decreases.

When methods such as atmospheric pressure chemical ionization−mass spectrometry (*4*, *5*) and proton transfer reaction−mass spectrometry (*6*) became available, it was possible to measure the effect of fat on flavor delivery during consumption. A series of in vivo studies of the consumption of foods with different fat contents showed that differences between products in vitro are not reproduced in vivo (*3*, *7*−*14*). In each case the differences in in vivo delivery between a low-fat and a high-fat sample were less than those that would be expected from static headspace measurements (*1*). These differences between the two techniques (in vivo and static headspace) can be substantial. Shojaei et al. (*14*) showed a difference in in vivo flavor delivery of 2.1-fold for ethyl hexanoate between high- and low-fat milk samples, whereas a factor of around 15-fold would be expected on a static headspace basis.

The differences observed between static headspace and in vivo delivery are due to the dynamic nature of in vivo delivery affecting mass transfer (*15*). There is a strong relationship between the air/product partition coefficient and the efficiency of in vivo flavor delivery. A decrease in the partition coefficient is accompanied by an increase in the efficiency of flavor delivery (*15*). This offsets the effect of fat on flavor partitioning, reducing the impact of fat on flavor delivery (*16*).

The many studies of the effect of fat on in vivo flavor delivery provide a database of values that can be used for modeling flavor behavior. The objective of this paper is to develop a predictive, empirical model of the effect of fat on in vivo flavor delivery. Key parameters for model development were the fat contents of the samples themselves and the log *P* of the flavor compounds (the log of the octanol/water partition coefficient), which is considered to be a reasonable approximation to the oil/water partition coefficient.

MATERIALS AND METHODS

Emulsion Preparation. Sucrose stearate (E-473) (Sisterna SP70, S. Black Ltd., Herts, U.K.) was dispersed in bottled mineral water (Deeside, Royal Deeside, Scotland; purchased from a local supermarket) using a low-shear mixer (Yellow Line OST 20 Basic) for 30 min. The water and sucrose stearate dispersion was then heated to 50 °C on a hot plate (Fisher Scientific Heated Magnetic Stirrer FB15001, Loughborough, U.K.) while being stirred with the low shear mixer. Once at 50 °C, the rapeseed oil (deodorized rapeseed oil, Florin, Switzerland; provided by Nestlé) was added and blended using a high-shear blender (Silverson Machines Ltd., Chesham, U.K.) for 15 min. This pre-emulsion was passed twice through a two-stage valve homogenizer (Panda 2k, Niro Soavi S.P.A., Sheffield, U.K.) fitted with a heated reservoir at 50 °C, at pressures of 500 bar (first stage) and 50 bar (second stage). The final emulsion contained 40% fat and 1% sucrose stearate. This emulsion was diluted with water to give a range of fat contents to which a series of flavor compounds were added.

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Compounds Used. Nonan-2-one, pyrazine, 3-methylbutanol, limonene, cymene, heptan-2-one, and ethyl nonanoate were purchased from Aldrich (Gillingham, Dorset, U.K.), purity ≥97%. Pyrazine and 3-methylbutanol were added to all emulsions (0, 1, 3, 8, 15, 22, 30, and 40% fat) at a concentration of 50 mg/L. The remaining compounds were added to water at 10 mg/L and to emulsions at 50 mg/L.

Flavor Release Studies. Three replicate samples (10 g) of each of the flavored emulsions were consumed by two panelists only. Simultaneously, their breath was sampled (30 mL/min) into an atmospheric pressure chemical ionization source fitted to a Platform II mass spectrometer (VG, Manchester, U.K.) through a heated (120 °C) deactivated fused silica transferline 1 m × 0.53 mm i.d. The source was heated to 75 °C and operated in positive ion mode (4 kV) at a cone voltage of 18 V.

Data were collected in selected ion recording mode with a dwell time of 0.02 s monitoring *m*/*z* 143, 81, 71, 137, 134, 115, and 187 for nonan-2-one, pyrazine, 3-methylbutanol, limonene, cymene, heptan-2-one, and ethyl nonanoate, respectively. Masslynx 3.2 (Micromass, Manchester, U.K.) was used to determine the peak height of the maximum signal observed for each sample. The differences in flavor release between samples were calculated on the basis of the average peak height ratios of samples with different fat contents, allowing for any differences in flavor volatile concentration.

Sensory Analysis. *Triangle Test*. Single cream purchased from a local supermarket (19.4% fat) was diluted with water and sugar (also purchased from a local supermarket) added to give a final emulsion that contained 1% fat and 5% sugar. This was flavored with either the high or low level of orange flavor mixture added at 0.15% (**Table 1**). A panel of 21 untrained panelists was presented with three samples labeled with three-letter codes, each set of three samples consisting of two samples at one flavor level and one at the other. The panelists were asked to taste the samples and decide which sample was different from the other two in a forced-choice experiment. The panelist's response was recorded and statistical analysis performed using Fizz software (ver. 2.00, Biosystemes, Couternon, France).

Modified Duo-Trio Test. Single cream purchased from a local supermarket (19.4% fat) was diluted with water and sugar (also purchased from a local supermarket) added to give a final emulsion that contained 1 or 10% fat and 5% sugar. The 10% fat emulsion was flavored with the high level of orange flavor and the 1% fat emulsion with either the high or low level of flavoring, all at 0.15%. Consequently, there were two samples with identical flavor addition and one different. Forty untrained panelists were presented with the three samples labeled with three-letter codes. The panelists were asked to taste the samples and decide which of the 1% fat emulsion samples was the most similar in flavor to that of the 10% fat emulsion sample in a forced-choice experiment. The panelist's response was recorded and statistical analysis performed using Fizz software.

Data Modeling. The effect of different lipid contents on the release of volatiles was modeled using Design Expert ver. 7.0.3 (Statease, Minneapolis, MN).

Log P Estimation. Log *P* was estimated using the KOWWIN program ver. 1.67 within EPISuite ver. 3.20 from the U.S. Environmental Protection Agency.

RESULTS AND DISCUSSION

Model 1: Existing Data. The range of data available for modeling the effect of fat on in vivo flavor delivery varies not only in the matrices and the equipment used for the analysis, but in the number of panelists and the degree of replication (*3*, *7*−*14*). The quality of the measure of intrasample differences should increase with greater replication and panelist numbers. In one instance (*14*), 98 panelists made four replicate assessments of the in vivo differences in ethyl hexanoate delivery from low-fat and high-fat milk, a total of 392 replicate assessments to produce one estimate of the effect of fat on flavor delivery. This approach should provide high-quality data for modeling, but would be too time-consuming for the generation of a large database of values.

The majority of the data available is based on far fewer panelists and replicates. However, in model development, it is generally better to have a wider range of data varying in sample type, flavor compound, and fat content than a higher degree of replication and panelist number, which often limits this diversity. This results in a broader model with wider applicability.

Table 1. Amounts of Compounds (Milligrams) Combined To Make either a Low- or High-Flavor Formulation[a]

compound	low	factor	high
hexanal	18.8	1.5	28.2
octanal	9.4	2.8	26.3
decanal	4.7	4.9	23.0
ethyl hexanoate	11.8	2.9	34.2
linalool	23.5	4.2	98.7
β-ionone	2.4	4.0	9.6
trans-p-menthane-8-thiol-3-one	2.4	2.0	4.8
ethyl butyrate	50	1.5	75
limonene	2000	3.8	7600

[a] The ratio between them (factor) was calculated by substituting the appropriate log *P* and fat content values into eq 3 and then calculating the ratio between the two release predictions. Each formulation was made up to 10 mL with ethanol. All compounds were supplied by Aromco (Royston, U.K.).

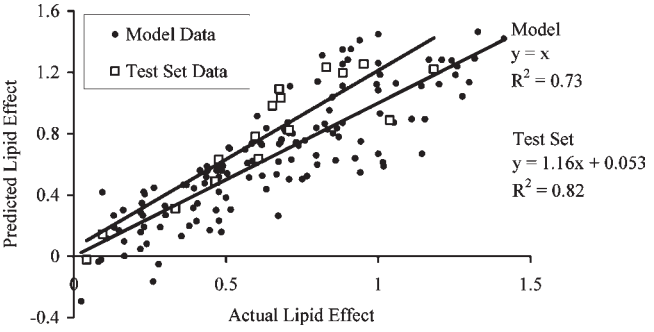

Figure 1. Actual and predicted lipid effect for the initial data set, which comprised a modeling set of 129 values and a test set of 16 values (eq 2).

Data from the literature (*3*, *7*−*14*) and a small amount of unpublished work (release differences for eight compounds in 3 and 22% fat mayonnaise) were combined, and a lipid effect (LE) value was calculated (eq 1)

$$\text{lipid effect (LE)} = \text{flavor delivery FC2/flavor delivery FC1} \quad (1)$$

where FC2 is the fat content (%) of the higher fat content sample and FC1 is the fat content (%) of the lower fat content sample.

The lipid effect values were modeled using Design Expert from Statease (based on multiple linear regression), using three values, log *P*, FC1, and FC2. A total of 129 data points were used for the development of the model with an additional 16 separate values used as a test set to check the predictive power of the model. Potential modeling terms were either kept in the model or excluded, on the basis of the statistical significance of their contribution to the model, such that terms with a probability of $P < 0.05$ were retained. The equation generated (eq 2) had 10 terms in addition to the intercept, including interactive terms between the three factors and quadratic and cubic components.

$$\begin{aligned} \text{LE} = {} & 1.35 - 0.093 \times \log P + 0.11 \times \text{FC1} - 0.062 \times \text{FC2} + \\ & 0.027 \times \log P \times \text{FC1} - 0.0096 \times \log P \times \text{FC2} - 0.0046 \times \\ & \text{FC1} \times \text{FC2} - 0.11 \times \log P^2 + 0.0054 \times \text{FC2}^2 + 0.019 \times \\ & \log P^3 - 0.00011 \times \text{FC2}^3 \end{aligned} \quad (2)$$

Table 2. Data and Model Predictions (Based on Equation 2) of the Impact of Changing Lipid Content (from Fat Content 1 to Fat Content 2) for the Test Set Compounds

compound	log *P*	FC1 (%)	FC2 (%)	actual lipid effect	predicted lipid effect[a]
diacetyl	−1.34	0	0.033	0.83	1.23
ethanol	−0.31	0.2	10	1.18	1.22
butan-2-one	0.29	0	1	0.95	1.25
butan-2-one	0.29	0	15	0.88	1.20
benzaldehyde	1.48	0	3.8	0.71	0.82
ethyl butyrate	1.85	2.7	3.8	0.68	1.09
heptan-2-one	1.93	0	5	0.48	0.63
heptan-2-one	1.93	2.5	5	0.65	0.98
heptan-2-one	1.93	5	15	0.68	1.03
3-methylbutyl acetate	2.25	0.5	30	0.33	0.31
ethyl pentanoate	2.34	3	22	0.61	0.64
ethyl hexanoate	2.83	5	15	0.60	0.78
octanol	3.00	5	10	1.04	0.89
nonan-2-one	3.14	2.5	10	0.46	0.49
ethyl octanoate	3.81	0	5	0.10	0.14
menthyl acetate	4.39	0	8	0.04	−0.02

[a] Predicted from model.

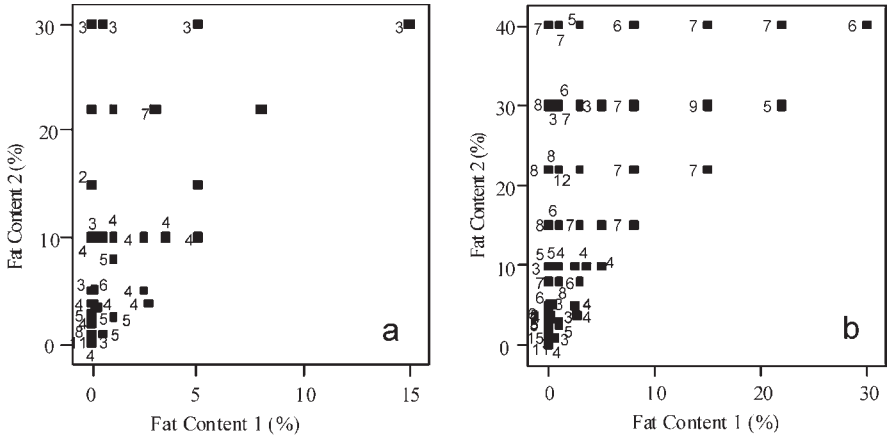

Figure 2. Distribution of experimental points for the initial modeling (**a**) and the final data set (**b**) with respect to the fat contents of the different samples. The numbers indicate multiple samples occurring at the same two fat contents; these are either replicates or compounds with different log *P* values.

The values obtained from eq 2 correlated with the modeling data set with an R^2 of 0.73 (**Figure 1**), which is reasonable given the diverse origins of the data set and the fact that it is formed of in vivo flavor delivery measurements. There is, however, the possibility with such complex modeling exercises to generate an equation that correlates with the data set but has no real predictive value. Consequently, the model was also used to predict a test set of LE values not previously used in the modeling exercise. The test set was predicted with an R^2 of 0.83, but the regression line had a slightly higher slope and intercept than that of the original model (**Figure 1**; **Table 2**). This demonstrated that the model had some predictive power and was not simply a spurious statistical correlation.

Overall, it appeared that it had been possible to model the data in one global model, despite its diverse origins. No one data set stood out as different from the rest, which would have indicated significant differences between the values reported by different research groups.

Development of Model. The model (eq 2) was limited by the range of sample fat contents included in the data set with few values at higher fat contents. **Figure 2a** shows the distribution of data points plotted as a function of the FC1 and FC2 dimensions. The data points are further spread by the third dimension, log *P*. In the FC2 dimension, there are only 12 values with an FC2 of 30%, whereas at an FC2 of 22%, 7 of the 10 values occur at just one value of FC1. Equally in the FC1 dimension there are only four values at an FC1 pf > 5%.

Clearly the data density at higher fat contents is limiting the strength of the model and its range of applicability. Models are usually best in the middle of the experimental design space (e.g., at mid log *P* values) where trendlines are supported by surrounding data. They are weakest around the periphery (extremes of log *P*), where there are fewer supporting data. Additional data were generated over a range of fat contents (0, 1, 3, 8, 15, 22, 30, and 40%) using a series of compounds with different log *P* values (**Figure 2b**). Three replicates of each fat content/compound combination were consumed by two panelists to generate a total of 200 new data points. The degree of replication and the number of panelists were limited but compensated for by the range of new values added across the experimental design space. This was particularly true for the higher fat contents, which were not adequately represented in the data obtained from the literature (**Figure 2a**). It was hoped that broadening the range of lipid contents and increasing data density at the extremes would make the model more robust.

Model 2: New and Old Data. The modeling exercise was repeated with the new data set, which now comprised 310 values for the model itself and 35 separate values that were used as a test set. The equation that was generated (eq 3) was similar to that of the first model in the range of modeling

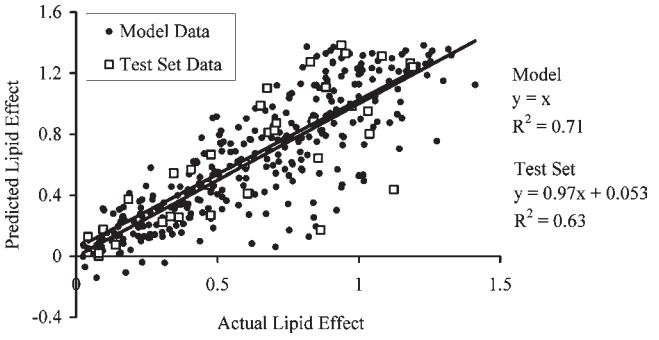

Figure 3. Actual and predicted lipid effect for the final data set, which comprised a modeling set of 310 values and a test set of 35 values.

terms included, with a total of 14 terms in addition to the intercept.

$$\begin{aligned} LE = {} & 1.41 + 0.082 \times FC1 - 0.037 \times FC2 - 0.11 \times \\ & \log P - 0.0069 \times FC1 \times FC2 + 0.052 \times FC1 \times \\ & \log P - 0.011 \times FC2 \times \log P + 0.0019 \times FC2^2 - 0.13 \times \\ & \log P^2 - 0.00071 \times FC1 \times FC2 \times \log P + 0.00012 \times FC1 \times \\ & FC2^2 - 0.0041 \times FC1 \times \log P^2 + 0.0023 \times FC2 \times \\ & \log P^2 - 2.7E-05 \times FC2^3 + 0.023 \times \log P^3 \end{aligned} \quad (3)$$

The correlation (**Figure 3**) between the actual modeling data and the values predicted by eq 3 was again reasonable (R^2 = 0.71), given the diversity of the data and potential variation in analytical measurements. The results of the test set had a slightly lower R^2 (0.63) but showed a slope and intercept close to that of the $y = x$ model equation, showing that this model also had good predictive power and was not a spurious statistical correlation (**Figure 3**; **Table 3**).

The model has three dimensions FC1, FC2, and log *P*. The effect of log *P* on in vivo flavor delivery can be seen by plotting the effect of the two fat contents at different values of log *P* (**Figure 4**). In **Figure 4a** the LE at a log *P* of 0.0 is shown. The lower right sector is grayed to show there are no data in this part of the design space because FC2 was always greater than FC1. The values near the lines on the contour plots show the LE values predicted by eq 3 across the design space. In the case of **Figure 4a** the values are around 1 with few contours, showing little effect of fat content on flavor delivery of compounds with a log *P* of 0.0, which is what might be expected.

As the log *P* is increased to 1.75, compounds become more hydrophobic and values near the contour lines decrease, showing an increased LE. The lowest values on the contour lines are at low values of FC1 and high values of FC2. This is consistent with the greatest difference in flavor release occurring between the lowest fat contents (FC1) and the highest (FC2). When both FC1 and FC2 had high lipid contents, there were smaller changes in flavor delivery (upper right sector of **Figure 4b**). This shows that there is less effect of increasing fat content on in vivo flavor delivery if there is already some fat present. Increasing log *P* to 4.0 (**Figure 4c**) showed the same trends as observed at a log *P* of 1.75; the lipid effect was, however, more pronounced.

Along the FC1 = FC2 line there are contour values of > 1.0, suggesting more release from a second sample with a slightly higher fat content than the first. In this particular part of the design space there are no data values (**Figure 2b**) that result in this phenomenon. A series of values (LE = 1) could have been added in for a range of FC1 = FC2 data points with different log *P* values. This would have weighted the trendline at FC1 = FC2 toward a value of 1.0, effectively comparable to forcing a trendline through the origin on a standard two-dimensional graph. These values were not included because these values would be artificial and not experimentally generated and as such lacked true experimental variation.

Table 3. Data and Model Predictions (Based on Equation 3) of the Impact of Changing Lipid Content (from Fat Content 1 to Fat Content 2) for the Test Set Compounds

compound	log *P*	FC1 (%)	FC2 (%)	actual lipid effect	predicted lipid effect
diacetyl	−1.34	0	0.033	0.83	1.27
ethanol	−0.31	0.2	10	1.18	1.27
pyrazine	−0.06	1	3	0.94	1.38
pyrazine	−0.06	3	40	1.08	1.31
pyrazine	−0.06	30	40	1.19	1.24
butan-2-one	0.29	0	1	0.95	1.33
butan-2-one	0.29	0	15	0.88	1.11
3-methylbutanol	1.16	1	15	0.70	0.82
3-methylbutanol	1.16	8	22	1.03	0.95
benzaldehyde	1.48	0	3.8	0.71	0.87
ethyl butyrate	1.85	2.7	3.8	0.68	1.10
heptan-2-one	1.93	0	5	0.48	0.66
heptan-2-one	1.93	0	30	0.18	0.37
heptan-2-one	1.93	2.5	5	0.65	0.99
heptan-2-one	1.93	3	22	0.35	0.54
heptan-2-one	1.93	5	15	0.68	0.81
heptan-2-one	1.93	22	30	0.98	0.98
hexenyl acetate	2.25	0.5	30	0.33	0.26
ethyl pentanoate	2.34	3	22	0.61	0.41
ethyl hexanoate	2.83	5	15	0.60	0.60
octanol	3.00	5	10	1.04	0.80
nonan-2-one	3.14	0	30	0.08	0.00
nonan-2-one	3.14	2.5	10	0.46	0.47
nonan-2-one	3.14	3	22	0.30	0.23
nonan-2-one	3.14	22	30	0.84	0.88
ethyl octanoate	3.81	0	5	0.10	0.17
cymene	4.10	0	15	0.08	0.02
cymene	4.10	3	8	0.41	0.57
cymene	4.10	15	30	0.86	0.64
ethyl nonanoate	4.30	1	3	1.12	0.44
ethyl nonanoate	4.30	3	40	0.14	0.08
menthyl acetate	4.39	0	8	0.04	0.13
limonene	4.48	0	3	0.36	0.25
limonene	4.48	1	30	0.86	0.17
limonene	4.48	8	40	0.48	0.27

In **Figure 3** it is clear that there were some major outliers in both the model data set and the test set. One of these is for a limonene test set sample, as the fat content varied form FC1 = 1.0 to FC2 = 30. The actual experimental data point was a LE of 0.86 compared with a predicted lipid effect from eq 3 of 0.17. The other main test set outlier was ethyl nonanoate as fat increased from 1 to 3%, for which the predicted LE was 0.46 compared with an actual measured value of 1.12. Either the model has predicted these values poorly or they are examples of experimental error (poor actual values). An increase in the delivery of ethyl nonanoate with increased fat was certainly not expected, because this compound is hydrophobic (log *P* = 4.30) and this is not in line with the vast majority of the data. These results are most likely outliers in the actual values, which might be expected with a data set of 345 values.

It would be very tempting to strip off the outliers observed in **Figure 3** and focus on the core of the data; however, that is a poor scientific practice. The poor values in one direction should be balanced by others in the opposite direction, with the model lying between. This highlights the possible benefits of a model rather

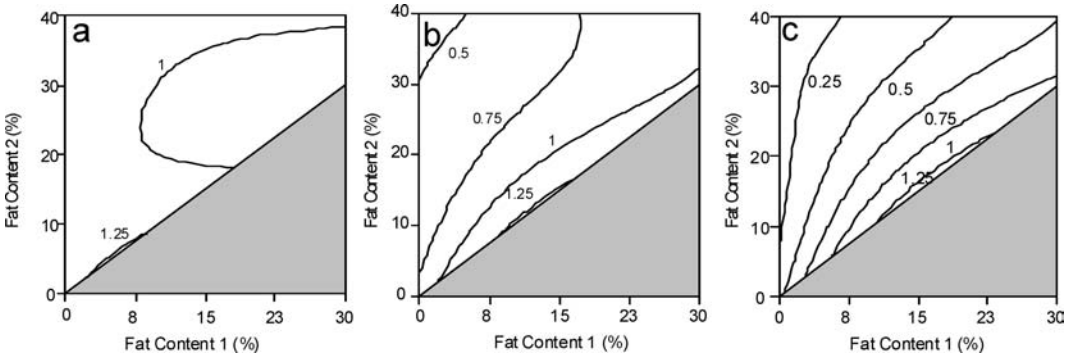

Figure 4. Effect of differences in lipid content on in vivo volatile release predicted by the fat content and log *P* model at three log *P* values: (**a**) 0.0; (**b**) 1.75; (**c**) 4.0. The model (eq 3) was based on 310 data points.

than actual measurements. The model gives a prediction based on the averages of a body of data, whereas making a measurement to find the actual value is in itself inherently associated with error.

The LE value with the greatest level of replication (392 replicate values for 98 panelists) showed an actual LE of 0.48 for ethyl hexanoate when 3.8% fat milk was compared with 0.1% fat milk (*14*) (see the Supporting Information). The predicted value in this case was 0.42, showing close agreement between experimentation and model prediction.

In addition to experimental and modeling error, there is the potential error in values such as log *P*, which is in itself the product of a model. The log *P* value used in this modeling exercise was from EPISuite, which is available from the U.S. Environment Protection Agency free of charge. The log *P* predictions from this model correlated closely ($R^2 = 0.86$) with experimental oil/water partition coefficient measurements (*17*). This combined with its availability made it the log *P* source of choice. There may be some potential for including other modeling terms in the LE models; however, there may be modeling limitations due to experimental variation in the data set. In addition, other models such as those for estimating the air/water partition coefficient may be associated with greater errors. The models of log *P* are potentially the most researched and robust, due to the pharmaceutical industries interest in log *P* for modeling drug uptake. They are also the most applicable to modeling changes in in vivo flavor delivery because they numericize the hydrophobicity of molecules.

Few data on the effect of fat in flavor reformulation have been published. One example of reformulating between high- and low-fat ice creams is given by Cheetham (*18*). There is no supporting information on the models used or method of flavor release assessment allowing further evaluation. Equation 3 was used to predict the reformulation differences described for the 0 and 15% fat content products. The plot of these values with those published shows a reasonable correlation (**Figure 5**) with two clear exceptions. These differences are due to differences in log *P* estimation. EPIsuite (used to calculate the log *P* values for the current models) typically gave estimates of log *P* higher than those listed in Cheetham (*18*), except for the two outliers, both of which had lower EPIsuite log *P* values than those originally published. This emphasizes the reliance of the lipid effect model on the quality of the log *P* model. It also highlights the fact that when a log *P* value is used in a model equation, it is important to obtain it from the same source as those used to generate the original model.

All of the lipid effect data used during the modeling exercise were from liquid or semiliquid samples. There are few results for more solid food systems such as baked goods. Dimelow (*19*) measured the in vivo release of flavor compounds from a baked crumb coating and the amount of flavor retained during the

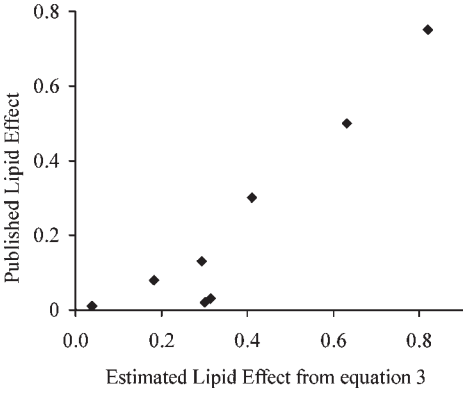

Figure 5. Relationship between the estimated lipid effect from eq 3 with published formulation differences for low-fat (0%) and high-fat (15%) vanilla ice cream (*18*).

baking process. Correcting for flavor losses, the LE values for anethole, pinene, and carvone for high-fat (7%) and low-fat (0.4%) crumb samples were all similar, 0.24, 0.24, and 0.25, respectively. The differences predicted for these compounds between 7 and 0.4% fat systems using eq 3 would be 0.23, 0.20, and 0.30, respectively. Similarly, Brauss (*8*) studied anethole release from high-fat (18%) and low-fat (4%) biscuits, finding a LE of 0.23 (after correction for losses during baking) compared with a model prediction of 0.35. Clearly, the measured lipid effects are similar to those predicted by the model (eq 3). However, a larger data set would be needed to fully evaluate the use of the model for solid food systems.

During the modeling exercise, no attempt was made to compensate for difference in fat particle size, largely because it is unknown and undefined for the majority of the data set. There will have been a variation in droplet sizes over the data set and the model could be thought of as taking the average line through this variation also. Few studies have examined the effect of droplet size on in vivo delivery. Linforth (*15*) did find differences in delivery of factors of 2.6 and 1.7 for ethyl hexanoate and octanol in lipid emulsions that had either been crudely blended or homogenized at high pressure, with less release from the crudely homogenized sample. This gives some idea about how much influence this might have on flavor delivery.

A further factor not taken into account during model development was the emulsifier itself. There may be interactions between the emulsifier and aroma compounds in emulsified systems, either nonspecifically, as a result of the physical properties and concentration of the emulsifier, or through chemical reaction.

Further advances in log *P* estimation may produce better quality values for modeling. The current data set is available

from the authors for future researchers to use with improved terms or additional modeling factors to try and develop the model further.

Application of the Model. One of the challenges for the food industry is the reformulation of flavors between products with different fat contents, to give a similar flavor delivery to the consumer. This can rely on sensory assessments or models such as eq 3, or each compound can be measured to give a guide to reformulation. Often scientists prefer measurements over models, but measurements can also be associated with errors. A high level of replication can minimize this. However, this is time-consuming, the equipment required is expensive, and some flavor compounds have such low odor thresholds that they will be unpalatable at concentrations at which they can be detected.

A flavor reformulation study was carried out using an orange flavor that was selected because it contained a high proportion of hydrophobic compounds; delivery during consumption will vary with fat content. Diluted cream was chosen as a simple real-world emulsion system, and this was diluted to give fat contents of 1 and 10%, both of which had a similar appearance (compared with a sample with 0% fat).

Table 1 shows the two levels of the orange flavor formulation and the reformulation factor between them. According to eq 3, the high level of flavor in the high-fat product should give the same flavor delivery as the lower flavor level in a low-fat product. The differences in flavor delivery were investigated sensorially.

In the first experiment, a triangle test was used to confirm that the there was a perceivable difference in orange flavor intensity or character when the two formulations were applied to just one sample matrix. The 1% fat system was used for this test because it represented the target product. If panelists could not detect the difference between the two flavor formulations in the cream taste/aroma background, then there would be little point in further flavor reformulation.

Twenty-one untrained panelists carried out a triangle test to see if they could tell the difference between the low- and high-flavor formulations in the 1% fat system. Twelve of the 21 were able to identify the sample with the different flavor level. This was statistically significant ($P = 0.021$), demonstrating that the two flavor formulations delivered perceivably different experiences. An untrained panel was selected for both this and the following sensory test to reflect the discrimination of typical consumers.

Following this, a duo-trio test was carried out, to see which of the two 1% fat samples (the one with the lower or the one with the higher flavor level) was perceived as most similar to the 10% fat system with the original high-flavor level. Of 40 panelists, 26 judged that the 1% fat sample with the lower flavor level was the most similar of the two to the 10% fat sample with the higher flavor. This was statistically significant ($P = 0.40$), demonstrating that the reformulated flavor in the lower fat product was indeed a closer match to that of the original.

The models and the reformulation study were based on in vivo peak height data rather than area data. The shape of the release profile (area/height ratio) will, however, have varied between samples of different fat contents dependent on the log P of the compound. The ability of the peak height model to estimate the reformulation assessed sensorially may indicate that the maximum intensity of aroma release (peak height) is more important to perception than the shape of the profile.

No model is ever perfect, but the final model (eq 3) does appear to have a capacity for predicting flavor delivery differences, draws together diverse sets of data, and may provide a tool in flavor reformulation. The model applies to high- and low-fat foods with data covering a wide range of log P values and fat contents. The systems were, however, typical of many experimental systems, fluid and reasonably homogeneous. Although the model appeared to show a good prediction of the effect of fat in two solid sample types, insufficient data were available for a true validation of the model with solid food systems. Consequently, the applicability of the model for solid foodstuffs is less certain. In solid food systems, fat may exist in solid, liquid, or, crystalline forms, and there may also be phase separation. Such factors are likely to exert further influences on flavor delivery.

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Supporting Information Available: Table of lipid effect values. This material is available free of charge via the Internet at http://pubs.acs.org.

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