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A polynomial regression model for the response of various accelerating techniques on maize wine maturation

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Abstract

Statistical analysis was conducted to interpret the recently observed effects of various accelerating techniques on maize wine maturation (Chang, A. C. (2004). The effects of different accelerating techniques on maize wine maturation. *Food Chemistry*, *86*, 61). Instead of the previously reported simple linear relationship between the concentrations of the key components of maize wine in the final product and the number of treatments or the dosage, various types of non-linear behaviours were observed. A general polynomial regression model is used to describe these behaviours, and the adjustable parameters were estimated from the experimental data. The performance of the proposed regression model, which plays a key role in the design of an efficient accelerating process, was satisfactory. Some specific variations of the key components of maize wine, as a function of the number of treatments or the dosage, were observed.

Keywords: Accelerating techniques; Maize wine; Maturation; General polynomial regression model

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1. Introduction

Wine aging is one of the key steps for improving the overall quality of wines. Reported methods for wine aging include those of a chemical nature (e.g. Huang, 1980; Sato, 1984; Simpson & Miller, 1983) and of physical nature (e.g. Cocito, Gaetano, & Delfini, 1995; Hua, Chen, Yu, & Huang, 1989; Lindley & Mason, 1987; Matsuura, Hirotsune, Nunokawa, Satoh, & Honda, 1994; Saterlay & Compton, 2000; Suslick, 1989). While the latter attracted less attention than the former, it is of practical importance since the aging period can be shortened considerably. Like chemical aging methods, physical aging methods can have a profound influence on the properties of wine. This is because treatments such as ultrasonic waves and irradiation may trigger complicated biochemical reactions, thereby leading to compositions that are significantly different from those without treatments, which implies that a comprehensive study of the influence of a treatment on the nature of wine is complex. This difficulty can be circumvented, as a first step, by examining the energy input on the concentrations of the key components of the final product. Chang and Chen (2002), for example, reported the effects of numbers of treatments of 20 kHz ultrasonic waves on the properties of rice and maize wines. Their analysis was extended by Chang (2004) in a recent study, where the effects of various accelerating techniques on maize wine maturation were investigated. Twenty kilohertz and 1.6 MHz ultrasonic and γ-irradiation treatments were applied, and the titratable acidity and the concentrations of the key components of maize wine in the final product (including alcohol, acetaldehyde, ethyl-acetate, 2-phenyl-ethanol, 1-propanol, 2-methyl-1-propanal, 2-methyl-butanol, and 3-methyl-butanol)

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were measured and compared with those of a one year conventionally matured wine. Most of the above-mentioned key components were found to correlate with the number of treatments/dosage and, based on a regression analysis, it was concluded that they are linearly dependent, that is, a simple linear model is applicable. Although it is empirical, this conclusion is of practical significance since it provides relationships that are necessary for the design of an accelerating process. However, a close examination of the data reported (Chang, 2004), plotted in Figs. 1–3 for illustration, reveals that the relationship between the dependent and the independent variables can be non-linear. Fig. 1, for example, shows that the concentration of 2-phenyl-ethanol seems to decay roughly exponentially with the number of treatments of 20 kHz ultrasonic waves. The curve for ethyl acetate in Fig. 2 shows a concave downward trend. Fig. 3 suggests that a quadratic relationship seems to ex-

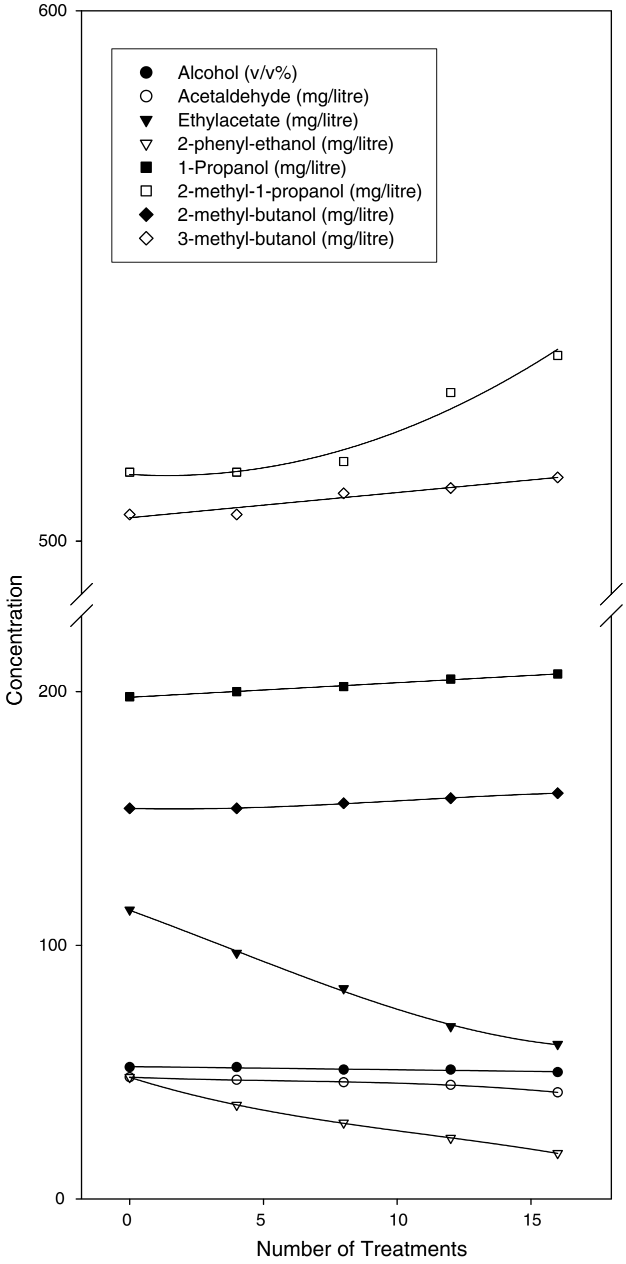

Fig. 1. Variation of the concentrations of the key components of maize wine, in the final product, as a function of the number of treatments for the case of 20 kHz ultrasonic wave-treated maize wine. Discrete symbols, experimental data (Chang, 2004); curves, results based on the models shown in Table 1.

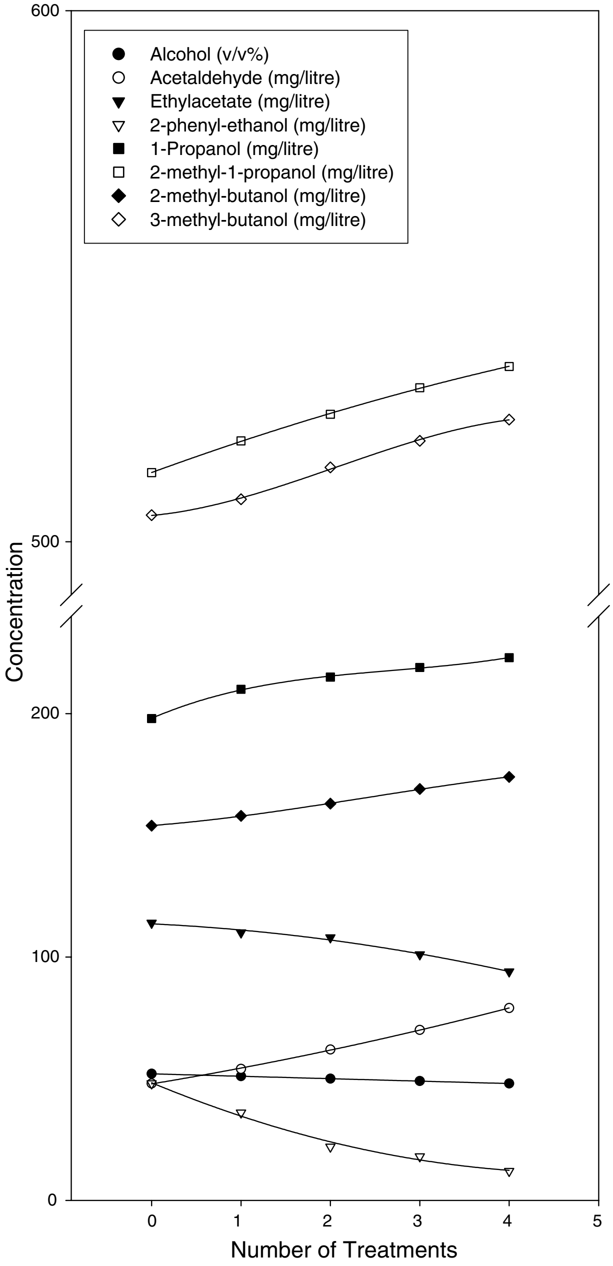

Fig. 2. Variation of the concentrations of the key components of maize wine, in the final product, as a function of the number of treatments for the case of 1.6 MHz ultrasonic wave-treated maize wine. Discrete symbols, experimental data (Chang, 2004); curves, results based on the models shown in Table 2.

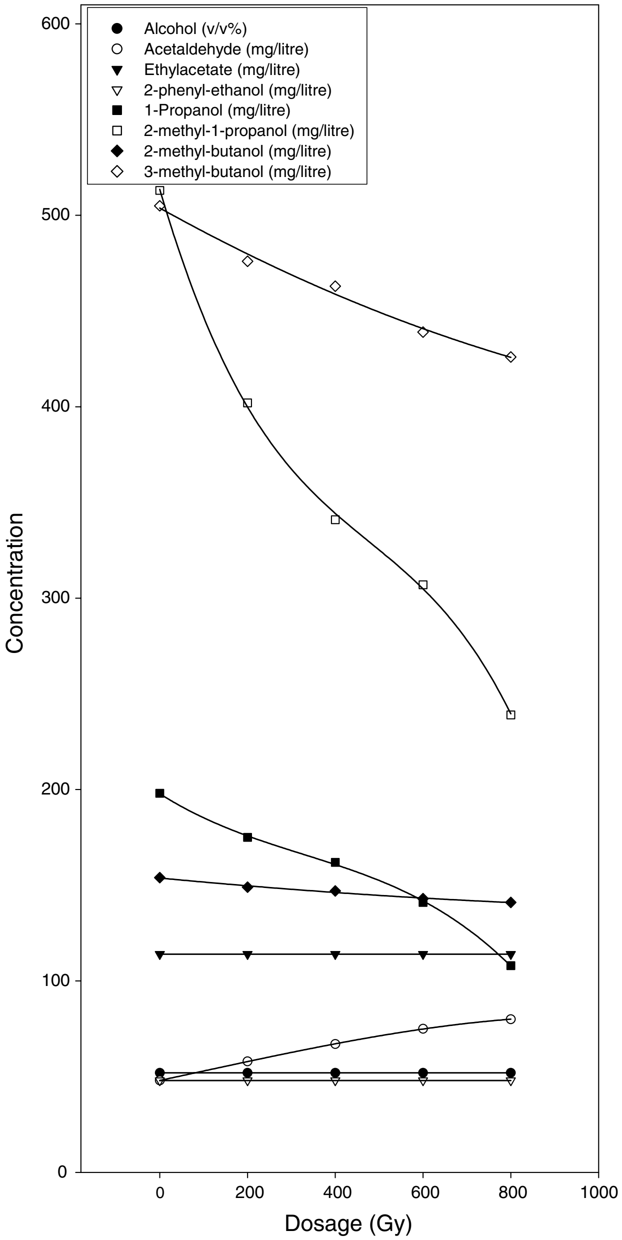

Fig. 3. Variation of the concentrations of the key components of maize wine, in the final product, as a function of dosage for the case of γ-irradiation treated maize wine. Discrete symbols, experimental data (Chang, 2004); curves, results based on the models shown in Table 3.

ist between the concentration of acetaldehyde and the dosage of γ-irradiation treatments. These observations imply that, to serve as potential accelerating techniques, a more detailed quantitative analysis of their performance is highly desirable. In this note, the experimental data of Chang (2004) are statistically reanalyzed, and empirical relationships that correlate the key components of maize wine with the number of treatments/dosage of an accelerating technique are built.

2. Data fitting procedure

Since an explicit relationship between the dependent variable Y, which represents the key components of maize wine (in the final product), and the independent variable X, which represents the number of treatments or the dosage, is unknown at the present stage, we consider a general polynomial model

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \cdots + \beta_k X^k + \varepsilon, \tag{1}$$

where β_i, $i = 0,1,2,\ldots,k$, are adjustable parameters and ε is a normal random variable with mean 0 and constant standard deviation σ. Eq. (1) can be viewed as an approximate relationship between Y and X, as long as Y can be expanded as a Taylor series in terms of X. Note that if $\beta_i = 0$ for $i = 2,\ldots,k$, then Eq. (1) reduces to that assumed by Chang (2004). The selection of the value of k is such that the adjusted coefficient of multiple determination, R^2_{Adjusted}, defined below, is maximized (Montgomery, Runger, & Hubele, 2004):

$$R^2_{\text{Adjusted}} = 1 - (1 - R^2)\left(\frac{n-1}{n-p}\right), \tag{2}$$

where p is the number of adjustable parameters, and R^2 is the coefficient of determination defined by

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}. \tag{3}$$

In this expression, $\bar{y} = \sum_{i=1}^{n} y_i/n$ and $\hat{y}_i$ are, respectively, the averaged value of the experimentally observed values of y and the ith value of y predicted by Eq. (1) based on a set of estimated parameters ($\beta_0,\beta_1,\ldots,\beta_k$).

3. Results and discussion

The result of the model building procedure is summarized in Tables 1–3, and the values of the key components of maize wine (in the final products), for various accelerating treatments predicted by the fitted models, are plotted in Figs. 1–3. In general, the agreement between the experimental data and the estimated values is reasonably good. The results presented in Tables 1–3 suggest that, for most of the key components, a simple linear relationship between their concentrations and the number of treatments/dosage is unsatisfactory; a quadratic or higher order relationship is more appropriate. As mentioned previously, the present polynomial model, Eq. (1), is an approximation of the true functional relationship. For instance, although the concentration of 2-phenyl-ethanol in Fig. 2 decays roughly exponentially with the number of treatments of 1.6 MHz ultrasonic waves, it can be described roughly by a quadratic function, as illustrated in

Table 1
Summary of model building procedure on the experimental data of Chang (2004) for the case of 20 kHz ultrasonic waves, Y and X are, respectively, the concentrations of the key components of maize wine, in the final product, and the number of treatments

Components	Regression model $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \cdots + \beta_k\ \mathrm{x}^k$
Alcohol (v/v%)	$Y = 5.220 \times 10 - 1.255 \times 10^{-1} X$
Acetaldehyde (mg/l)	$Y = 4.803 \times 10 - 4.226 \times 10^{-1} X + 4.464 \times 10^{-2} X^2 - 2.604 \times 10^{-3} X^3$
Ethyl acetate (mg/l)	$Y = 1.138 \times 10^2 - 3.836X - 7.143 \times 10^{-2} X^2 + 6.510 \times 10^{-3} X^3$
2-Phenyl-ethanol (mg/l)	$Y = 4.797 \times 10 - 3.327X + 1.741 \times 10^{-1} X^2 - 5.208 \times 10^{-3} X^3$
1-Propanol (mg/l)	$Y = 1.978 \times 10^2 + 5.744 \times 10^{-1} X$
2-Methyl-1-propanol (mg/l)	$Y = 5.126 \times 10^2 - 3.107 \times 10^{-1} X + 1.116 \times 10^{-1} X^2$
2-Methyl-butanol (mg/l)	$Y = 1.540 \times 10^2 - 2.440 \times 10^{-1} X + 8.036 \times 10^{-2} X^2 - 2.604 \times 10^{-3} X^3$
3-Methyl-butanol (mg/l)	$Y = 5.044 \times 10^2 + 4.750 \times 10^{-1} X$

Table 2
Summary of model building procedure on the experimental data of Chang (2004) for the case of 1.6 MHz ultrasonic waves, Y and X are, respectively, the concentrations of the key components of maize wine, in the final product, and the number of treatments

Components	Regression model $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \cdots + \beta_k\ \mathrm{x}^k$
Alcohol (v/v%)	$Y = 5.200 \times 10 - 1.000X$
Acetaldehyde (mg/l)	$Y = 4.786 \times 10 - 6.086X + 4.286 \times 10^{-1} X^2$
Ethyl acetate (mg/l)	$Y = 1.136 \times 10^2 - 1.7571X - 7.857 \times 10^{-1} X^2$
2-Phenyl-ethanol (mg/l)	$Y = 4.834 \times 10 - 1.529 \times 10^1 X + 1.571X^2$
1-Propanol (mg/l)	$Y = 1.981 \times 10^2 + 1.577 \times 10^1 X - 4.7143X^2 + 5.833 \times 10^{-1} X^3$
2-Methyl-1-propanol (mg/l)	$Y = 5.130 \times 10^2 + 6.143X - 2.857 \times 10^{-1} X^2$
2-Methyl-butanol (mg/l)	$Y = 1.540 \times 10^2 + 2.810X + 1.214X^2 - 1.667 \times 10^{-1} X^3$
3-Methyl-butanol (mg/l)	$Y = 5.049 \times 10^2 + 1.548X + 2.071X^2 - 3.333 \times 10^{-1} X^3$

Table 3
Summary of model building procedure on the experimental data of Chang (2004) for the case of γ-irradiation, Y and X are, respectively, the concentrations of the key components of maize wine, in the final product, and the dosage

Components	Regression model $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \cdots + \beta_k\ \mathrm{x}^k$
Alcohol (v/v%)	$Y = 52$
Acetaldehyde (mg/l)	$Y = 4.803 \times 10 + 4.905 \times 10^{-2} X + 5.357 \times 10^{-6} X^2 - 2.083 \times 10^{-8} X^3$
Ethyl acetate (mg/l)	$Y = 114$
2-Phenyl-ethanol (mg/l)	$Y = 48$
1-Propanol (mg/l)	$Y = 1.978 \times 10^2 - 1.458 \times 10^{-1} X + 2.250 \times 10^{-4} X^2 - 2.292 \times 10^{-7} X^3$
2-Methyl-1-propanol (mg/l)	$Y = 5.135 \times 10^2 - 7.839 \times 10^{-1} X + 1.252 \times 10^{-3} X^2 - 8.750 \times 10^{-7} X^3$
2-Methyl-butanol (mg/l)	$Y = 1.538 \times 10^2 - 2.171 \times 10^{-2} X + 7.143 \times 10^{-6} X^2$
3-Methyl-butanol (mg/l)	$Y = 5.038 \times 10^2 - 1.275 \times 10^{-1} X + 3.750 \times 10^{-5} X^2$

Table 2. This is because the exponential relationship $Y = a\exp(bX)$ can be expanded as

$$Y = a\exp(bX) = a\left[1 + bX + \frac{(bX)^2}{2!} + \cdots\right]. \tag{4}$$

Therefore, if (bX) is sufficiently small, since higher order terms can be neglected, this expression reduces to the form

$$Y \cong \beta_0 + \beta_1 X + \beta_2 X^2. \tag{5}$$

Similar arguments apply to other types of non-linear relationships. We have to emphasize that, due to the limitation of the number of available data, searching for a more realistic and physically sounder quantitative relationship between the concentrations of the key components of maize wine (in the final product) and the number of treatments/dosage is not feasible at the present stage, and further study is necessary. Nevertheless, the empirical relationships presented in Tables 1–3 are capable of describing, quantitatively, the relationship between the dependent and the independent variables, which can be used directly in the design of an accelerating process.

Figs. 1–3 show several interesting trends. For example, Fig. 1 suggests that, for the case of 20 kHz ultrasonic-wave treatments, the concentration of acetaldehyde declines roughly linearly with the number of treatments when it is less than 12, and starts to decline faster after that. The concentration of ethyl acetate becomes insensitive to the number of treatments when it exceeds about 16. Both the variation of the concentration of 2-methyl-1-propanal and that of 3-methyl-butanol, as a function of the number of treatments of 20 kHz ultrasonic waves, are of sigmoidal nature; the former is insensitive to the number of treatments when it is below 6 or above 18, and the latter is insensitive to the number of treatments when it is below 4 or above 14. As can be seen in Fig. 2, the variation of the concentration of 3-methyl-butanol, as a function of the number of 1.6 MHz ultrasonic wave treatments, also shows a sigmoidal trend. The concentration of 2-phenyl-ethanol decays roughly exponentially with the number of treatments for both 20 kHz and 1.6 MHz ultrasonic wave treatments, as illustrated in Figs. 1 and 2. The curve for ethyl acetate, for 20 kHz treatments, is of a concave upward nature, but the reverse is true for 1.6 MHz treatments. The curve for the concentration of acetaldehyde, in the case of 20 kHz ultrasonic wave treatments, also has a reverse trend compared to that in the case of 1.6 MHz ultrasonic wave treatments. Fig. 3 shows that the qualitative behaviour of the curve for 1-propanal is similar to that of 2-methyl-1-propanol; both show an inflection point near 400 Gy. The concentration of 3-methyl-butanol decays roughly exponentially with the dosage of γ-irradiation treatments. In contrast, it increases with the number of treatments in the case of ultrasonic wave treatments, as shown in Figs. 1 and 2. Similar to the case of 1.6 MHz ultrasonic wave treatments, the concentration of acetaldehyde increases with the dosage of γ-irradiation treatment. However, the curve for the former is of a concave upward nature, but the latter is of a concave downward nature.

It should be pointed out that the regression relations, summarized in Tables 1–3, should be used for interpolations only; that is, they are applicable for predicting the value of the dependent variable when the value of the independent variable is in the range which is used to construct the regression relations. Extrapolations, which may lead to unrealistic results, are not suggested (Montgomery et al., 2004). For instance, if γ-irradiation is applied, then according to Table 3, the concentration of 2-methyl-1-propanol will become negative if the dosage is sufficiently large, which, of course, is meaningless.

4. Conclusion

In summary, we show that the effects of ultrasonic-wave and γ-irradiation treatments on maize wine maturation are of a complicated nature. In particular, the concentrations of the key components of maize wine in the final product, can exhibit various non-linear relationships with the number of treatments/dosage. These relationships are essential for the design of an efficient accelerating process.

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References

Chang, A. C. (2004). The effects of different accelerating techniques on maize wine maturation. *Food Chemistry, 86*, 61–68.

Chang, A. C., & Chen, F. C. (2002). The application of 20 kHz ultrasonic waves to accelerate the aging of different wines. *Food Chemistry, 79*, 501–506.

Cocito, C., Gaetano, G., & Delfini, C. (1995). Rapid extraction of aroma compounds in must and wine by means of ultrasound. *Food Chemistry, 2*, 311–320.

Hua, F. M., Chen, Q. F., Yu, Y. T., & Huang, L. G. (1989). Acceleration of yellow rice wine mellowness by cobalt ray. *Acta Agriculture Nucleatae Sinica, 3*, 178–186.

Huang, C. C. (1980). *Studies on the chemical aging method of Shaoshing wine*. Annual Report of Wine Factories of the Taiwan Tabacco and Wine Monopoly Bureau. Taiwan.

Lindley, J., & Mason, T. (1987). Sonochemistry-synthetic applications. *Chemical Society Review, 16*, 275–311.

Matsuura, K., Hirotsune, M., Nunokawa, Y., Satoh, M., & Honda, K. (1994). Acceleration of cell growth and ester formation by ultrasonic wave irradiation. *Journal of Fermentation and Bioengineering, 77*, 36–40.

Montgomery, D. C., Runger, G. C., & Hubele, N. F. (2004). *Engineering statistics* (third ed.). New York: John Wiley & Sons.

Saterlay, A. J., & Compton, R. G. (2000). Sonoelectroanalysis-an overview. *Fresenius Journal Analytical Chemistry, 367*, 308–313.

Sato, S. (1984). *Aging of foods*. Japan: Japanese Kung Ling Press.

Simpson, R. F., & Miller, G. C. (1983). Aroma composition of aged Riesling wine. *Witis, 22*, 51–63.

Suslick, W. H. (1989). The techniques of wine sensory evaluation. *Techniques of wine produce-Taiwan Tobacco and Wine Monopoly Bureau, 2*, 40–57.