THERMAL DIFFUSIVITY ESTIMATION FROM THERMAL PROCESS DATA

By

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ABSTRACT

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Error analysis of the analytical solution to the Fourier heat conduction equation used in estimating thermal diffusivity from thermal process data is presented. The influence of the following factors on the nonlinear regression estimation of thermal diffusivity were investigated: 1) misplacement of the temperature measurement probe, 2) variations in container dimensions, 3) measurement error in time and temperature, 4) assumption of an infinite surface heat transfer coefficient when finite values are present, 5) violated boundary conditions related to factors such as come-up time and head space, and 6) heat conduction along the temperature measurement probe.

A Monte-Carlo analysis of a mathematical model, along with actual thermal process data collected for water thickened with sodium-calcium alginate, revealed that thermal diffusivity calculated from heat penetration data is largely dependent on errors associated with temperature measurement and to a lesser extent dependent on errors in

thermocouple probe location. Errors in temperature measurement consisted of both random errors and those arising from heat conduction along the temperature measurement probe. Can dimensions and time measurement errors had a minor influence on the estimation of thermal diffusivity. Heat conduction along the temperature measurement probe resulted in large and autocorrelated errors that could be compensated for with the use of a quasi-steady state solution for heat conduction along a cylinder (probe).

Best thermal diffusivity prediction accuracy is obtained using the following guidelines: 1) use a totally filled can, 2) use as large a can as possible, 3) use a can with a length over diameter ratio close to 0.8, 4) maintain the difference between the initial and heating medium temperature above 40 deg C, 5) use only the data collected between the temperature ratio range of 0.15 to 0.85, 6) establish the magnitude of the correction factor needed to compensate for heat conduction along the temperature measurement probe, 7) establish the magnitude of the Biot Number for the surface of the can or maintain it above 200, 8) accurately measure the time, can dimensions, and position of the temperature measurement probe, and 9) examine the residuals of the estimate for unsatisfied boundary conditions. Estimating thermal diffusivity from the slope (f_h) of the heat penetration data may result in poor estimates and is not a recommended practice.

To God the Father and Jesus Christ, without whom all wisdom of the world is as striving after wind.

> "For the word of the cross is to those who are perishing foolishness, but to us who are being saved it is the power of God. For it is written,
>
> > 'I will destroy the wisdom of the wise,
> > And the cleverness of the clever I will
> > set aside.'
>
> Where is the wise man? Where is the Scribe? Where is the debater of this age? Has not God made foolish the wisdom of the world?"
>
> (I Corinthians 1:18-20;
> New American Standard)

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SYMBOLS

A = surface area of cylinder (m^2)

Bi = Biot Number

C_v = coefficient of variance (σ/μ)

f_h = inverse slope of heat penetration curve (hr)

F_o = thermal death time at 250 deg F

Fo = Fourier number

h = surface heat transfer coefficient ($W/m^{2\circ}C$)

j_h = intercept for time zero of heat penetration curve

J_0 = zero order Bessel Function of the first kind

J_1 = first order Bessel Function of the first kind

k = thermal conductivity ($W/m^{2\circ}C$)

L = half height of can or half thickness of an infinite slab (m)

m' = probe factor (m^{-1}, $\sqrt{hP/Ak}$)

P = perimeter of cylinder (m)

r = radial position in can (m)

R = radius of can or radius of an infinite cylinder (m)

S = estimate of standard deviation

SR = sensitivity coefficient ratio (equation 9)

t = time (hr)

T = temperature (°C)

x = axial position in can (m)

$\bar{x}$ = estimate of mean

Subscripts

a = actual

b = bottom

c = calculated

i = initial or index number

m = medium

n = index number

s = side of can

t = top of can

Greek and Other

α = thermal diffusivity (m^2/hr)

β = roots of eigenfuction for cylinder

γ = roots of eigenfuction for nonsymmetrically heated slab

Θ = temperature ratio = $(T - T_m)/(T_i - T_m)$

λ = roots of eigenfuction for symmetrically heated slab

μ = mean of population

π = Pi the constant 3.14156

σ = standard deviation of population

ε = residual of mean $(\mu - \bar{x})$

∞ = infinity

RESEARCH OVERVIEW

RESAERCH OVERVIEW

Over the last few years a large number of heat conduction problems (Matthews and Hall, 1968; Teixeira et al., 1969; Teixeira et al., 1975a; Teixeira et al., 1975b; Lenz, 1977; Hayakawa, 1979; Saguy and Karel, 1979; Ohlsson, 1980; Naveh et al., 1983; Young et al., 1983; Naveh et al., 1984) have been investigated where an accurate value of thermal diffusivity (α) was an asset. Whenever the research (Teixeira et al., 1975; Ohlsson, 1980; Naveh et al., 1984) included an error analysis of the problem, it was observed that the precision of the thermal prediction was strongly dependent on having an accurate value of α. As long as solutions to heat conduction problems are dependent on accurate thermal parameters, estimation procedures for these variables need to be refined and improved.

Thermal diffusivity estimation procedures can be broadly grouped into four categories (Nesvadba, 1982; Singh, 1982): 1) heat pulse and line heat source methods, 2) direct use of temperature profiles to determine the physical properties, 3) temperature matching (or - least squares), and 4) regular regime (or phase) - use of linear portion of heating curve. With regard to thermal processing of cans or pouches, the estimation procedure for α that has been used the most is that of the regular regime method. The reason is due to the fact that the estimation of α can be done with just a few calculations by plotting heat penetration data on graph paper (Olson and Jackson, 1942); hence, there is no need for involved computer programming and analysis.

Simplicity and accuracy are both desirable attributes that should be taken into consideration when deciding on a method of estimating α. Even though the regular regime method is simple to use, its accuracy is very questionable. Teixeira et al. (1975a) measured α using two can sizes and came up with results that were different by over 15%. Hicks (1961) has observed f_h values that fluctuate as much as 13%, which results in fluctuations of α of almost the same amount. Thus, even though the regular regime method is simple and easy to use, the accuracy of the estimate can no longer be considered acceptable, taking into account newer methods of α estimation.

Since the advent of computers a number of the other estimation methods have become easier to use. It has been over twenty years since Beck's (1963) original paper concerning the suggestion of obtaining α through nonlinear regression of the temperature measurements, and very few researchers (Matthews and Hall, 1968; Ross et al., 1969; Hayakawa, 1971; Hayakawa, 1972; Hayakawa and Bakal, 1973; Lenz, 1977; Albin et al., 1979; Narayana and Murthy, 1981; Nesvadba, 1982; Young et al., 1983) have exercised this method for foods. Even fewer of these researchers (Lenz, 1977; Young et al., 1983) used nonlinear regression with thermal process data; however, neither of these papers considered the propagation of error in the estimated α value from data containing error. Considering the above, the objectives of this research were to:

1) Investigate the sources of error in the collection of thermal process data,
2) Investigate the influence of data error on the estimation of α using nonlinear regression,
3) Outline procedures to be used in estimating α from thermal process data,
4) Compare the accuracy and precision of obtaining α using nonlinear regression and using the regular regime method.

Chapter I

Model and Computer Simulated Analysis

Introduction

Thermal processing of food is required to inactivate harmful bacteria. During the processing of foods not only is the bacteria inactivated but the physical characteristics of the food product, such as the textural and nutritional properties, are altered. In recent years, interest in the thermal processing of foods has focused on the optimization of the physical properties by altering the processing time and temperature so bacteria is inactivated but the physical and nutritional properties are retained as well as possible (Matthews and Hall, 1968; Teixeira et al., 1969; Teixeira et al., 1975a; Teixeira et al., 1975b; Saguy and Karel, 1979; Ohlsson, 1980). The heat transfer calculations involved in these research projects were carried out using one of three methods: 1) an analytical solution to the heat conduction problem, 2) finite differences, and 3) finite elements. When the boundary conditions cause the problem to be nonlinear, then the latter two methods are the easiest to use, but when this is not the case — as in thermal processing — the analytical solution to the heat conduction problem is a reliable method.

No matter what calculation procedure is used, if a food processor is to perform optimization calculations the thermal properties of the food product need to be known. Since the food processor already has equipment to (and must) measure the thermal process (F_o) of a set of processing conditions, it seems reasonable to use the same equipment and thermal process data to obtain estimates of food thermal properties.

Factors that can affect accurate and precise estimations of thermal properties are: 1) thermocouple probe location, 2) error in measuring container size, 3) error in time or temperature measurement, 4) assumed infinite surface heat transfer coefficients when they are finite, 5) heat conduction down the thermocouple probe, and 6) unmet boundary conditions (come-up time, head space, etc.). The first four factors are best investigated using Monte Carlo simulation in conjunction with sensitivity analysis of the model, which is considered in this chapter. The latter two factors involve experimentation and will be addressed in Chapter II.

Literature Review

Methods of Diffusivity Estimation

With regard to foods, thermal diffusivity (α) has been a neglected thermal parameter, and few values for it have been published. In contrast, thermal conductivity has had a large number of values published (Woodams and Nowrey, 1968; Polley et al., 1980). This is probably due to the simple empirical relationship that α has with f_h in thermal process calculations. Also, since α is defined in terms of thermal conductivity, specific heat and density it can be calculated indirectly.

Methods of estimating α can be grouped into four general categories (Nesvadba, 1982; Singh, 1982): 1) heat pulse or heat source, 2) direct use of temperature profiles to determine the physical properties, 3) temperature matching, and 4) regular regime. Heat pulse and heat source methods usually entail a known heat source, either applied to the sample through the outside of the sample container or by the use of a probe inserted into the sample. Methods that have used the temperature profiles of heat penetration data use the data — a slope or individual point — in conjunction with an analytical solution to the problem. Methods that fall into the category of temperature matching may also involve the use of a known heat source; however, the principle attribute of the procedure is that of

minimizing the difference between the measured and predicted temperature of the process. Of all the categories, the last one has been the method of choice for a large number of research projects. The method of regular regime involves the estimation of α from the heat conduction data over long time periods, where the heat conduction curve follows a regular pattern (i.e., a straight line).

Diffusivity Using the Line Heat Source Method

The line heat source method (Sweat and Haugh, 1974; Baghe-Kahandam et al., 1981) has been used extensively in measuring thermal conductivity of foods. The method is simple and the thermal concutivity of most foods can be measured using a small probe. Nix et al. (1967, 1969) published a procedure that has extended the use of the thermal conductivity probe so both thermal conductivity and thermal diffusivity can be estimated simultaneously. This extended method has been used to analyze a number of food products (rapeseed, Moysey et al., 1977; squash and white potatoes, Rao et al., 1975; peanut pods, hulls, and kernels, Suter et al., 1975; cooked beef, Baghe-Kahandam and Okos, 1981; tomato juice, Choi and Okos, 1983). There are many benefits in using the line heat source method over other techniques: 1) the sample size can be small, 2) the duration of the test is short (usually less than 8 mins), 3) it can be used to measure the thermal properties over a small temperature range, 1-5 deg C, allowing for the measurement of the thermal properties as a function of temperature, and 4) the boundary conditions are usually easily satisfied. A 5% error in k and α is typical for the line heat source method. The only real disadvantage for a food processor is that thermal process data cannot be used to determine thermal property values. Instead, different experiments would need to be carried out.

Diffusivity Using Temperature Profiles

Flambert (1974) and Nevadba (1982) have presented two very novel ways of obtaining estimates of α. Flambert showed that the heat flux of a transient heat conduction problem would reach a maximum at a specific Fourier number (Fo), depending on the shape of the container (Fo = 0.12 for an infinite cylinder). Thus, by finding the time at which the heat flux was maximum, α can be calculated from the theoretical Fo value. Nevadba's estimation procedure is particularly useful for freezing food, because it takes into consideration the temperature dependence of the thermal properties. Nevadba used the peak (for freezing; valley for heating) of the temperature gradient curve as a function of time to estimate α. This caused a term in the differential equation to go to zero, making the differential equation easier to solve.

The biggest limitation to the above methods is that determination of the maximum (or minimum) is difficult and is usually done using curve fitting, which adds an additional amount of error to the data collection error already present. Nevadba's method involves a grid of thermocouples, which is not easily incorporated into a typical thermal process procedure. Flambert's method was originally investigated using thermal process data and results in using a single point to estimate α. This, in conjunction with the error of curve fitting in Flambert's method, does not make the technique compatable with the precision of the temperature matching methods.

Diffusivity Using Temperature Matching

A number of different temperature matching calculation procedures (nonlinear regression, direct grid search, and Newton-Raphson) have been used to reduce the difference between the measured temperature and that calculated by the proposed model. Nonlinear regression is by far the fastest and most versatile method. Grid searching becomes very involved as the number of independent variables increases, and the Newton-Raphson method is limited to only one variable. Nonlinear regression has been used in only a few research projects involving foods (Matthews and Hall, 1968; Ross et al., 1969; Albin et al., 1979; Narayana and Murthy, 1981). Several research projects involving foods have used one of the other procedures (Hayakawa, 1971; Hayakawa, 1972; Hayakawa and Bakal, 1973; Lenz, 1977; Young et al., 1983). Of these projects, only Lenz (1977) and Young et al. (1983) used thermal process data to back out a value for α.

Nonlinear regression is a method for data analysis, not data collection; thus, any data collection procedure can be used. For example, the line heat source method uses nonlinear regression when estimating both k and α at the same time. Thus, there are no inherent limitations to the use of nonlinear regression analysis. Limitations are solely dependent on the data collection procedure.

Diffusivity Using Regular Regime

In 1923 when Ball published the "formula" method, calculations of a thermal process where made considerably easier. This method has become a standard by which all other methods are compared. Expanding on the "formula" method, Olson and Jackson (1942) correlated the analytical solution to the heat conduction problem with the parameters of the "formula method" and showed that f_h is directly related to α after long time periods (Fourier Modulus; Fo less than 0.20, i.e., during the regular regime). This correlation has come to be known as the Olson and Jackson equation. For the most part, authors (Hicks, 1961; Teixeira et al., 1969; Annamma and Rao, 1974; Teixeira et al., 1975a; Teixeira et al., 1975b; Ohlsson, 1980; Rizvi et al., 1980; Peterson and Adams, 1983) have adopted Olson and Jackson's equation for estimating α. Even though Olson and Jackson's equation is easy to use, it is limited by assumptions: 1) infinite and constant surface heat transfer coefficient, 2) constant thermal properties, and 3) use of just the first term of an infinite series. A number of the authors listed above have found that when estimating α from f_h, errors in of 5% to 13% are not atypical.

Gaffney et al. (1980) made an extensive review of the use of the regular regime for estimating α, which also took into account the possibility of estimating finite surface heat transfer coefficients. The methods by which a finite surface heat transfer coefficient may be taken into account has been used in a number of different research projects (Bhowmik and Hayakawa, 1979; Domen, 1980; Uno and Hayakawa, 1980a; Arce et al., 1981; Marich and Bachlich, 1982; Poulsen, 1982). The paper by Uno and Hayakawa (1980a) even goes on to present a method by which the finite surface heat transfer coefficients for the top, bottom, and side of a finite cylinder can be estimated along with α; however, the usefulness of such a method is still to be shown for thermal process data. Before the above-mentioned research was done, correlations of j (the intercept of the heat conduction curve) with the surface heat transfer coefficient (h) were used for the estimation of h (Pflug et al., 1965). Since Pflug's et al. paper, reliability of the estimates obtained from j have come into question due to the large variation in j values that are obtained from thermal process data.

A rather specialized regular regime method was developed by Dickerson (1965). In this method, a constant change in temperature is applied to an infinite cylinder, and α is estimated from a simplified solution to the transient heat conduction equation. Dickerson's procedure has not received a lot of attention, but was used by Rizvi et al., 1980. Probably the main reason for its lack of use is that the technique requires special handling, i.e., a special cylinder and an environment that changes temperature at a constant rate with time.

Errors Involved in Diffusivity Estimation

When limiting the research to determine α from thermal process data, only three methods reviewed above are available for use: 1) Flambert's method (1974), 2) temperature matching using the analytical solution to the heat conduction problem, and 3) regular regime. Noting that the available precision of the regular regime ranged from 5% to 13% (Hicks, 1961; Teixeira et al., 1975a; Bhowmik and Hayakawa, 1979; Uno and Hayakawa, 1980a; Uno and Hayakawa, 1980b), it seemed that one of the other methods had to have better precision. When Flambert's method was reviewed it was pointed out that it involved curve fitting to obtain a maximum and so was considered unsuitable. Considering the flexibility of the temperature matching method — any theoretical model can be used (as long as there is a method of solution) — nonlinear regression is the best method of choice. Before nonlinear regression can be fully advocated, an indepth error analysis of the model to be used on the thermal process data must be carried out.

Nesvadba (1982), in a review of estimating α from foodstuffs, enumerated a number of different factors that can contribute to an error in the estimation of α. Nesvadba broke the potential errors into two categories: 1) systematic errors and 2) random errors. The systematic errors consisted of: 1) those related to the actual container or probe, not the theoretical geometry, 2) heat loss by conduction or radiation laterally, 3) conduction along the thermocouple leads, 4) distortion of the temperature profile due to the thermocouple, 5) finite surface heat transfer coefficient when assumed to be infinite, 6) anisotropy of the food, 7) moisture migration, 8) change in composition or structure due to heat or mass transfer, 9) temperature dependent thermal properties, 10) evaporative cooling, 11) instrument sampling errors, 12) positioning of thermocouple, 13) instrument calibration, 14) graphical techniques, 15) neglection of terms in the infinite series solution to heat conduction problem, 16) numerical solutions, and 17) curve fitting. The random errors were enumerated as: 1) initial boundary condition not met, 2) time-dependent boundary conditions, 3) contact resistance, 4) air inclusions, 5) moisture gradients, 6) nonhomogenous sample, 7) genetic and variety differences, 8) imprecise measurement of temperature, 9) electric noise, and 10) calculations by the experimenter.

Errors Important to Thermal Process Data

When using thermal process data not all of the potential errors that are specified above apply. Many of the errors that do apply are considered with assumptions only. Others are satisfied with proper experimental design. Since the resultant α value is to be used in various optimization programs, the assumptions stated in these programs will applied here. These assumptions are: 1) physical and thermal properties of the food products are not temperature dependent, 2) products are homogeneous, isotropic materials, 3) the foods are heated only by pure conduction, 4) the products have a uniform initial temperature, 5) environmental changes are instantaneous (i.e., no lag time in retort come-up), 6) surface heat transfer coefficients will consist of a lumped parameter; involving external surface convection, conduction in the container material, and internal contact resistance and, 7) there is no phase change in the product during heating.

From previous experiments, factors that have been shown to be important when estimating α from thermal process data are: 1) position of the thermocouple probe (Hayakawa, 1971; Hayakawa and Bakal, 1973; Bhowmik and Hayakawa, 1979; Narayana and Murthy, 1981), 2) dimensions of the container (Uno and Hayakawa, 1980; Narayana and Murthy, 1981), 3) unknown or finite boundary conditions (Bhowmik and Hayakawa, 1979; Gaffney et al., 1980; Uno and Hayakawa, 1980a; Arce et al., 1981), 4) measurement of temperature (Bhowmik and Hayakawa, 1979; Gaffney et al., 1980; Uno and Hayakawa, 1980a), 5) moisture migration during the analysis (Arce et al., 1981), and 6) heat conduction down the thermocouple probe (Ecklund, 1955; Cowell et al., 1959; Beverloo and Welding, 1969; Teixeira et al., 1975a; Gaffney et al., 1980).

Error in Thermocouple Position

Errors in the position of the thermocouple increase in importance as the ability to position it with respect to the thickness of the sample decreases. Narayana and Murthy (1981) found (with a sample thickness of 10mm) that an error in the position of the thermocouple of $\pm$ 0.2mm resulted in an error in the estimation of α of 1.1%. Likewise, Hayakawa and Bakal (1973) found that an error in the position of the thermocouple of $\pm$1mm resulted in an error in α of up to 30% for a sample 32.0 to 35.0mm thick. Hayakawa (1971) and Bhowmik and Hayakawa (1979) also mentioned that error in the position of the thermocouple affected the precision of the α estimation; however, they did not indicate the magnitude of the error.

Error in Can Dimensions

Errors in the calculation of dimensions of the container have not been cited by many researchers as an important factor in the estimation of α. Narayana and Murthy (1981) found it to be more important than the errors in position of the thermocouple. With errors of $\pm$ 0.2mm in the thickness of the slab, Narayana and Murthy found a 3.0 to 3.3% variation in α. Uno and Hayakawa (1980) mention dimensions of the container as a factor, but do not indicate any relative magnitudes. They do recommend using a container size as large as conveniently possible.

Error in Unmet Boundary Conditions

To explain the lack of precision in the estimation of thermal properties, one of the first factors that is investigated as the possible cause is that of unmet boundary conditions. Bhowmik and Hayakawa (1979) and Uno and Hayakawa (1980a) point out that just such an error can occur when the surface heat transfer coefficients (h) are neglected. They found that h may not be infinite (as commonly assumed) due to head-space in the can and retort packing effects. To correct for this, Bhowmik and Hayakawa (1979) developed a method using a long cylinder to estimate both α and h values. This was done by solving (using the regular regime) the analytical solution of heat penetration in an infinite cylinder with a finite surface h value. Then, from a heat penetration test they calculated α and h. In a similar fashion, Uno and Hayakawa (1980a) developed a procedure where α and h_i where i = t,b,s (h is finite and different on each side of a can; h_t = surface heat transfer coefficient for the top, h_b = surface heat transfer coefficient on the bottom, and h_s = surface heat transfer coefficient for the side) can be estimated from the actual heat penetration data of a canned product. In an error analysis of this latter method, errors of 1mm in location and dimensional quantities, 1 deg C in temperature, and 5% in f_h values were used to predict a maximum relative error value of 24.6% for α in a 300x409 can. An error of this magnitude renders this method of estimation undesirable even though the factors used to calculate the error were not unreasonable.

The need to take into consideration surface heat transfer coefficients for a thermal process is solely dependent on head-space and retort packing. Ramaswamy et al. (1983) measured h for a variety of steam qualities and found h values the order of 11,000 W/m^2C for 98% steam. For the lower limit of a Biot Number equal to 200 (Gaffney et al., 1980; error in α of 1%), an h value of 11,000 W/m^2C corresponds to a characteristic length of 1.25 cm (assuming $k = 0.682$ W/mC for water). Cans with a characteristic dimension smaller than 5.0 cm are almost never used; thus, if there is any surface resistance, it will come from head space or retort packing problems. Just such a condition was shown to exist with "crateless retorts" where the cans end is flat on the retort bottom (Naveh et al., 1984).

Bhowmik and Hayakawa (1979) and Uno and Hayakawa (1980a) lumped temperature and time measurement errors in with the ability to obtain precise values for f_h. Thus, the errors in the measurement of temperature or time have not been investigated with regard to a direct effect on the estimation of α. Gaffney et al. (1980) has indicated that data collection should terminate when the temperature difference between the heating media and the product falls below $1^{\circ}C$. The primary reason for this is that measurement precision decreases as the temperature difference decreases. Bhowmik and Hayakawa (1979) observed this effect because after long time periods, the plots of the temperature differences between the product and the heating media fluctuated significantly.

Arce et al. (1981) researched defatted soy flour and found that moisture migration is an important factor when estimating thermal properties. For dry materials, moisture migration during an analysis must be taken into consideration, but since thermal processing is done on foods that have water activity levels above 0.80, moisture migration is not a problem.

Second to unmet boundary conditions, the error associated with heat conduction down thermocouple leads is the most investigated cause for errors in the estimation of thermal properties. This problem is best analyzed from actual experimental analysis and thus will be discussed more fully in Chapter II.

Theoretical Development

The following were assumed for all models used in this analysis: 1) physical and thermal properties of the food products are not temperature dependent, 2) products are homogeneous, isotropic materials, 3) the food is heated by conduction, 4) the product has a uniform initial temperature, 5) environmental changes are instantaneous (i.e., no lag time in retort come-up), 6) surface resistance will consist of apparent h values associated with external surface convection, conduction in container material and internal surface convection and, 7) there is no phase change in the product during heating. In conjunction with these assumptions only the heating phase will be investigated.

Fourier's equation of heat conduction with no internal heat source for an infinite slab is

$$\frac{\partial^2 \theta}{\partial x^2} = \frac{1}{\alpha}\frac{\partial \theta}{\partial t} \tag{1}$$

The analytical solution (Özişik 1980) to equation (1) for a thickness of 2L, a surface heat transfer coefficient of h for the top and bottom of the slab, and origin at the center is

$$\theta = \frac{T - T_m}{T_i - T_m} = 2 \sum_{n=1}^{\infty} \left[\frac{\sin(\lambda_n)}{\lambda_n + \sin(\lambda_n)\cos(\lambda_n)}\right] \exp\left[\frac{-\lambda_n^2 \alpha t}{L^2}\right] \cos\left(\lambda_n \frac{\alpha}{L}\right) \tag{2}$$

with

λ_n = roots of $\lambda_n \tan\lambda_n$ = Bi

Bi = Biot number for the slab - hL/k

α = thermal diffusivity

x = distance from center

T_m = temperature of heating medium

T_i = uniform initial temperature of the slab, i.e., temperature at t = 0.0

t = time

T = temperature in the slab at time t and point x

satisfying the following initial and boundary conditions:

$$\theta = 1.0 \text{ when } t = 0.0$$

$$\frac{\partial\theta}{\partial x} = 0 \text{ when } x = 0.0$$

$$\frac{\partial\theta}{\partial x} = \frac{-h}{k}\,\theta \text{ when } x = L$$

When h is assumed infinite, θ = 0 at x = L, then equation (2) reduces to

$$\theta = \frac{4}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{(2n-1)}\cos\left(\frac{(2n-1)\pi x}{2L}\right)\exp\left[-\left(\frac{(2n-1)\pi}{2}\right)^2\frac{\alpha t}{L^2}\right] \quad (3)$$

Fourier's equation for heat conduction for an infinite cylinder with no internal heat source is

$$\frac{1}{r}\frac{\partial\theta}{\partial r} + \frac{\partial^2\theta}{\partial r^2} = \frac{1}{\alpha}\frac{\partial\theta}{\partial t} \quad (4)$$

The analytical solution (Özişik 1980) to equation (4) for a cylinder of radius R, having a surface heat transfer coefficient of h and the origin along the cylindrical axis is

$$\theta = 2 \sum_{n=1}^{\infty} \frac{1}{\beta_n} \frac{J_1(\beta_n) J_0\left(\beta_n \frac{r}{R}\right)}{J_0^2(\beta_n) + J_1^2(\beta_n)} \exp\left[\frac{-\beta_n^2 \alpha t}{R^2}\right] \tag{5}$$

with

β_n = roots of $\beta_n J_1(\beta_n) = (Bi) J_0(\beta_n)$

J_0 = Bessel Function of the first kind, of order zero

J_1 = Bessel Function of the first kind, of order one

r = distance from the center

$Bi = hR/k$

satisfying the following initial and boundary conditions:

$$\theta = 1.0 \text{ when } t = 0.0$$

$$\frac{\partial \theta}{\partial r} = -\frac{h}{k}\theta \text{ at } r = R$$

$$\frac{\partial \theta}{\partial r} = 0 \text{ at } r = 0.0$$

When h is assumed infinite, $\theta = 0$ at $r = R$, then equation (5) reduces to

$$\theta = 2 \sum_{n=1}^{\infty} \frac{J_0\left(\beta_n \frac{r}{R}\right)}{\beta_n J_1(\beta_n)} \exp\left[\frac{-\beta_n^2 \alpha t}{R^2}\right] \tag{6}$$

where β_n are the roots of $J_0(\beta_n) = 0$

The analytical solution (Uno and Hayakawa 1979; Özişik 1980) to equation (1) for a slab thickness of 2L, surface heat transfer coefficient for the top and bottom of h_t and h_b respectively, and origin at the bottom of the slab is

$$\theta = 2 \sum_{n=1}^{\infty} \exp\left[\frac{-\gamma_n^2 \alpha t}{4L^2}\right] \frac{(\gamma_n^2 + Bi_t^2)(\gamma_n \cos(\gamma_n x) + Bi_b \sin(\gamma_n x))}{(\gamma_n^2 + Bi_b^2 + Bi_b)(\gamma_n^2 + Bi_t^2) + Bi_t(\gamma_n^2 + Bi_b^2)}$$

$$\left[\sin(\gamma_n) + \frac{Bi_b}{\gamma_n}(1 - \cos(\gamma_n))\right] \tag{7}$$

with

$$\gamma_n = \text{roots of } \tan(\gamma_n) = \frac{(Bi_b + Bi_t)\gamma_n}{\gamma_n^2 - (Bi_b Bi_t)}$$

Bi_t = Biot number for top of slab, = $h_t 2L/k$

Bi_b = Biot number for bottom of slab, = $h_b 2L/k$

x = distance from bottom of slab

satisfying the following initial and boundary conditions:

$$\theta = 1.0 \text{ when } t = 0.0$$

$$\frac{\partial \theta}{\partial x} = \frac{h_b}{k}\theta \text{ at } x = 0$$

$$\frac{\partial \theta}{\partial x} = \frac{-h_t}{k}\theta \text{ at } x = 2L$$

The product of equation (5) or (6) and (2), (3), or (7) represents the heat transfer model used during this study. Equation combinations were selected depending on whether or not there was symmetric or nonsymmetric heating for the top and bottom of the can and/or if the surface heat transfer coefficient was assumed infinite, because less computer time was required for calculation of equation (6) than (5) and less time was required for the calculation of equation (3) than (2) or (7). Each of the above equations were written as FORTRAN-77 subroutines which could be used by any of the programs developed during the study.

Analytical Procedure

Five can sizes (307x409, 307x306, 307x512, 202x308, and 603x700) were selected for this investigation (Table 1). The first three can sizes were chosen for their constant radius, moderate size, and varying L/R ratios. Can sizes 202x308 and 603x700 were chosen to represent small and large cans often used in industry.

Table 1

Can sizes used in computer simulated error analysis

Can Number	Radius (R) (m)	Half Height (L) (m)	L/R
307x409	.04366	.05794	1.327
307x306	.04366	.04286	.982
307x512	.04366	.07303	1.673
202x308	.02699	.04445	1.647
603x700	.07858	.0889	1.131

The variables used for the Monte Carlo error analysis of the model consisted of: time(t), temperature (T), length dimension of the can size (2L), radius dimension of the can size (R), radial location of the thermocouple probe (r), axial location of the thermocouple (x), and surface heat transfer coefficients (h_i, where i = t, b, s). The problems related to surface heat transfer coefficients are not related to measurement error but come from assumptions drawn by the experimenter, i.e., most calculations assume h is infinite and uniform along the can, which is often incorrect. This is an error which one can account for knowingly in the model; therefore, errors associated with the assumption of h were analyzed after the other factors were investigated.

With the advent of microelectronics numerous data acquisition units have been produced that allow for very accurate and precise temperature and time measurements. In addition to increased precision, data-acquisition units' also eliminate human error associated with reading data off a chart-type recorders. Therefore, it was assumed that errors associated with time and temperature measurements were not a result of human variations but due solely to mechanical variations. Time variations (95% confidence interval) used in this study followed an autoregressive order with an error in time of $\pm$ .005% (t) $\pm$ 1 sec which is the case for the data acquisition system used in the experiments (Hewlett Packard Model 3045DL). For the temperature factor, copper-constantan thermocouples were assumed which, in the range of interest (20 - 130°C), produced a measurement error of the order of $\pm$ 0.5 to 1.0°C. Errors for probe location were made the same for each can and set to a 95% confidence interval for error related to $\pm$ 4.0 mm for the radial placement and $\pm$ 4.0 mm for the axial placement. Due to the high precision needed to ensure proper lid closure and seam formation, this work assumed two thousandths of an inch variations in can length and diameter, which results in a 95% confidence region of error equal to $\pm$ 0.5 mm for can length and diameter. Surface Biot Number variations ranged from 10 to infinity. A summary of errors (for a 95% confidence region) used in the measurement of the model conditions is listed in Table 2. Populations of normally distributed points were generated using the Box-Muller transformations on a set of pseudorandom numbers (Beck and Arnold, 1977). These points were then transformed using the mean and standard deviations of the specific parameter(s) under investigation to obtain normally distributed points from which the heat transfer model could be tested.

To analyze the error factors a set of calculated or "actual" data points were produced with α = .00062 m^2/h, h = ∞ , the thermocouple probe located at the center, and no errors in time, temperature or can dimensions. From each "actual" time data point used, a set of 150 points were generated with an assumed error factor. For each point generated a α value was calculated using a direct search method (Beck and Arnold, 1977) minimizing $(T_a - T_c)^2$ where T_a is equal to the actual temperature and T_c is equal to the calculated temperature. The initial product temperature and the medium temperature were set equal to 65.0 and 121.1°C respectively.

Table 2

Error factors used to generate computer simulated data containing error for the analysis of the analytical solution to Fourier's heat conduction equation.

Factor	Attribute Standard Deviation
Time	.000025 t ± 1 sec
Temperature	.3333 deg C
Can half length	.000125 m
Can radius	.000125 m
Probe location (axially)	.002 m
Probe location (radially)	.002 m
	Range
Surface Biot Number (Bi_t, Bi_b, and Bi_s)	10 to ∞

The mean and standard deviation was recorded for each set of 150 α values, with the standard deviation measured about the "actual" value of α (.00062 m^2/h). Each parameter (except Bi) listed in Table 2 was varied individually to test its effect on the heat transfer model. Then, all the parameters (except Bi) in Table 2 were varied at the same time.

From the combined effect of all the error factors (except Bi) of Table 2, a distribution of the mean and standard deviation of α was obtained with respect to temperature. From this error distribution a population of 20 temperature values were created for each known mean and standard deviation (50 values) of α, for nine different Bi values ranging from 10 to ∞. This gave 1000 points for each Bi number for a total of 9000 points. Thermal diffusivity values were calculated assuming an infinite h value such that $\sum_{i=1}^{1000} (T_{a,i} - T_{c,i})^2$, using nonlinear least squares (Moré et al., 1981), was minimized. Recall that T_a refers to points produced assuming α is equal to .00062 m^2/h and Bi is a value in the specified range (Table 2).

The same populations of data points discussed above were used to simulate a heat penetration test from which f_h values were calculated. Calculation of f_h values were carried out with a FORTRAN-77 subroutine which maximized the coefficient of determination (r^2) of the data by regressing the data for a specific number of points and then by regressing the data again with one less point (removing the smallest time value). The elimination of points was repeated until the data with one less point had a coefficient of determination lower than the one with one more point.

In addition to Monte Carlo simulation of the heat conduction model, the sensitivity coefficients (the derivatives of the model with respect to the coefficient in question) were analyzed (Beck and Arnold, 1977). Sensitivity coefficients, when used for analysis and when needed by the nonlinear regression program, were calculated using the forward difference method.

Results and Discussion

Error Analysis

Two statistics that are usually used to describe the distribution of populations are the mean (μ) and the standard deviation (σ). For ease of comparisons, the results of error analysis are described by the residuals of the mean ($\varepsilon = (\mu - \bar{x})$; where $\bar{x}$ = estimate of μ) and the coefficient of variance ($C_v = S/x * 100$; where S = estimate of σ). Plots of ε/μ and C_v versus Θ for each of the error factors are depicted in Figures 1 through 14. Note that Θ varies from one to zero with complete heating. From Figures 1,3,5,7, and 9 it can be seen that variations in thermocouple probe location, can dimension, and time result in low ε values for long time periods.

Error in Probe Location

Errors in thermocouple probe location result in ε values that are all positive (Figures 1 and 3) because the thermocouple probe was located at the slowest heating point of the can. Hence, an error in thermocouple probe location will always result in an underestimation of the actual values of α. The underestimation of α for an error in probe location is the largest for the can with the largest relative heat penetration rate and the smallest dimensions. This means that two factors influence the error associated

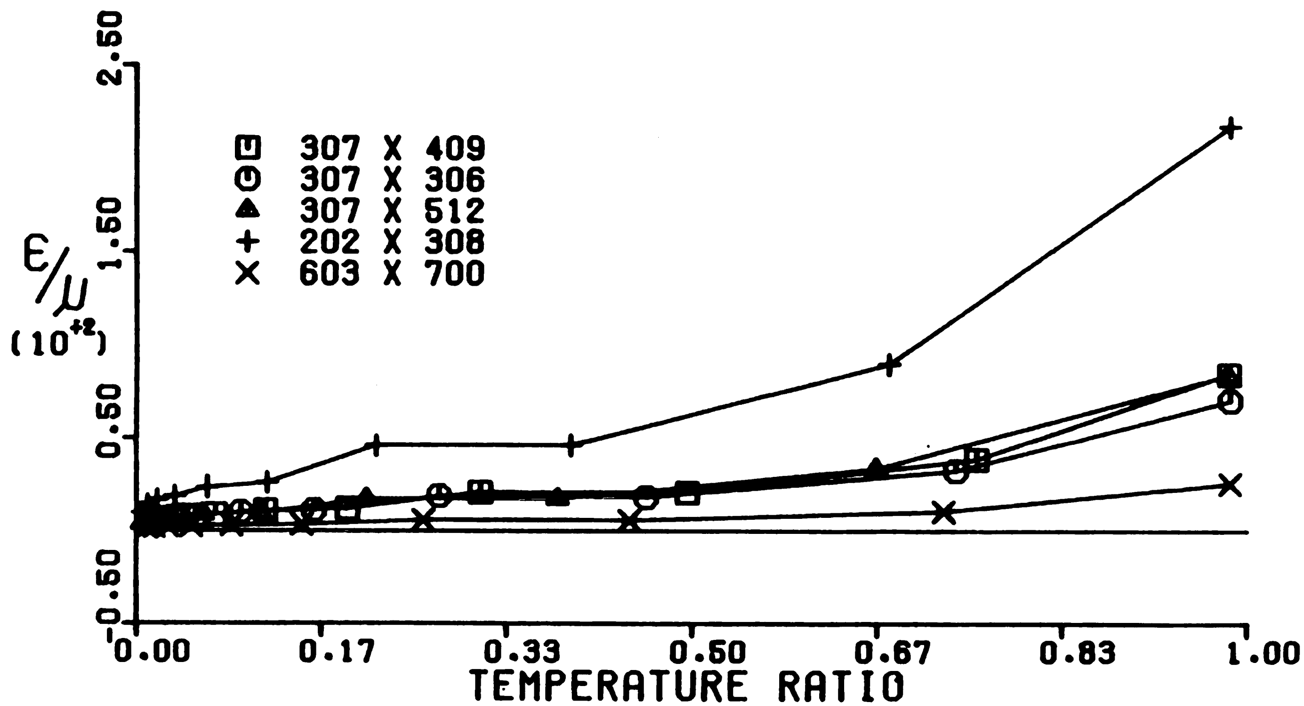

Figure 1. Residual error distribution for error in radial placement of thermocouple probe.

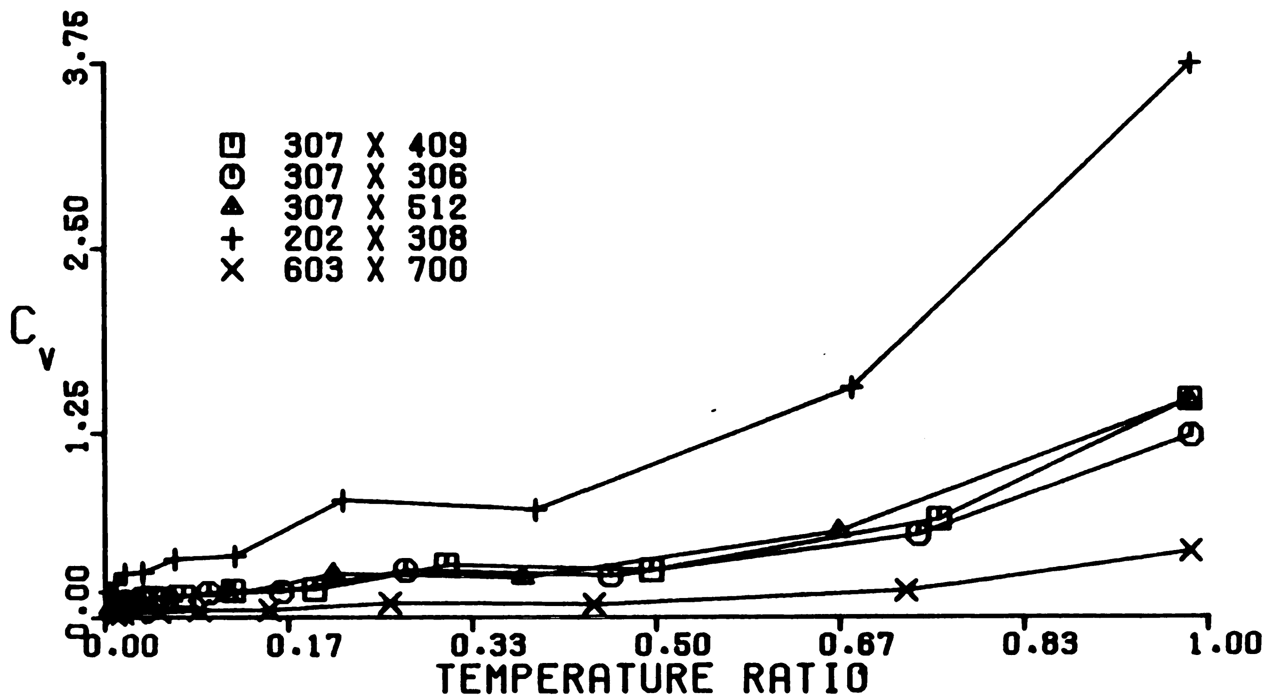

Figure 2. Variance distribution for error in radial placement of thermocouple probe.

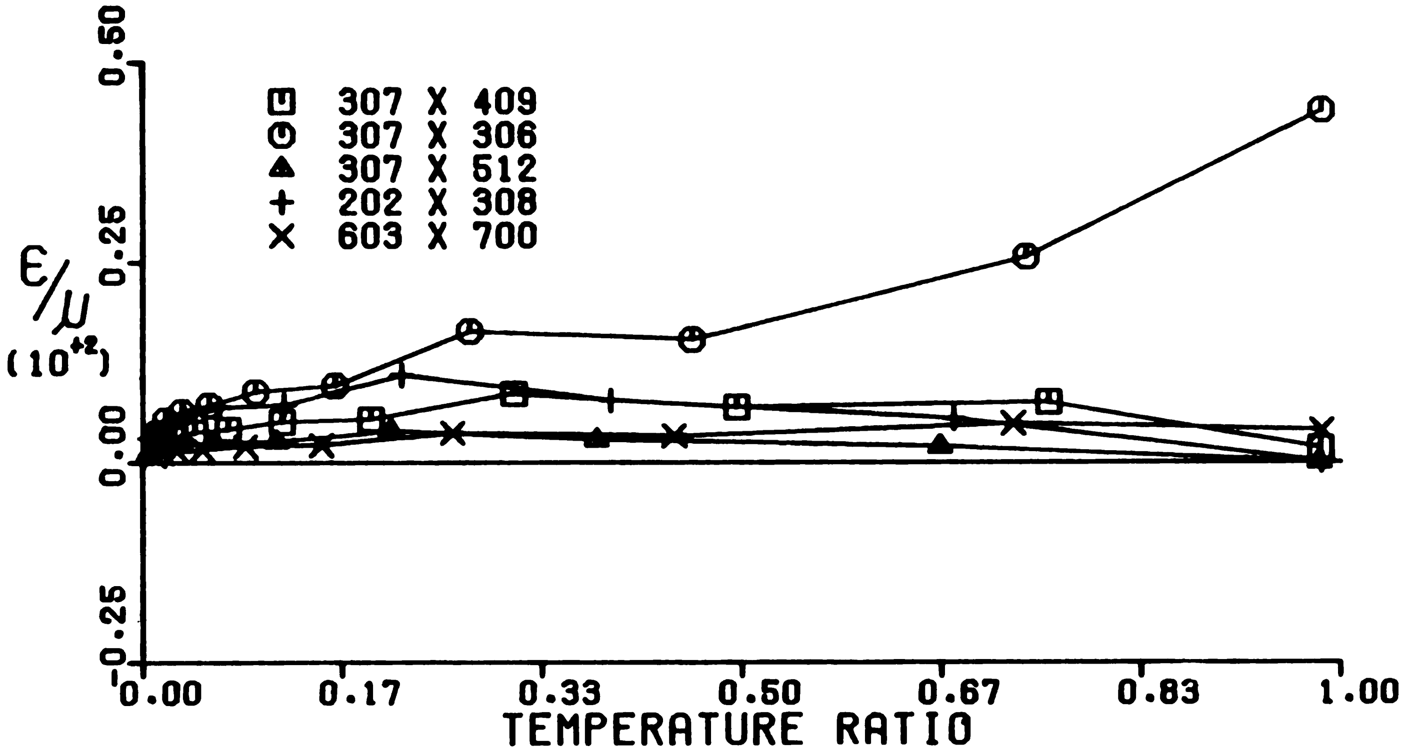

Figure 3. Residual error distribution for error in axial placement of thermocouple probe.

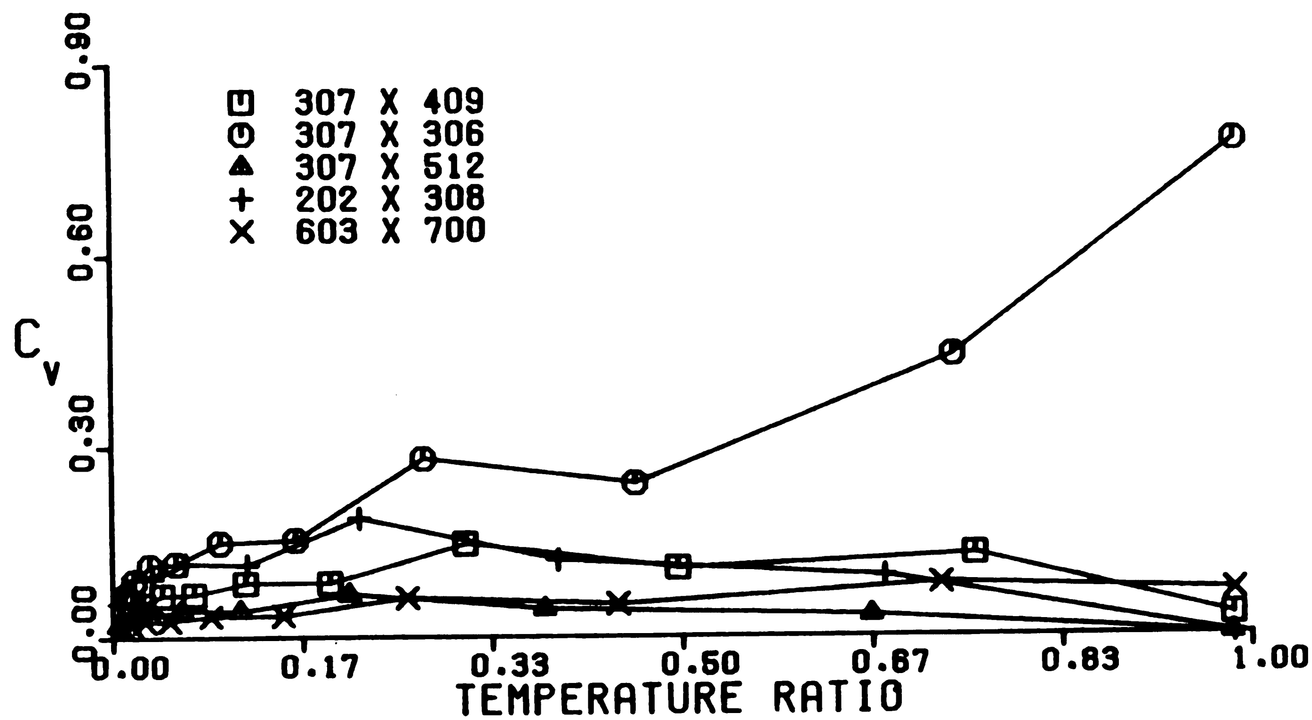

Figure 4. Variance distribution for error in axial placement of thermocouple probe.

with probe location. The first is the heat penetration rate for one dimension as compared with that of the other dimension (L/R). The second is the relative misplacement (r/R) of the thermocouple probe. For example, in the case of the 202x308 can the majority of the heat penetration is from the radial direction (i.e., a large L/R; Table 1). In addition, the 202x308 has a small radius, where the same displacement in thermocouple probe (in all the cans studied) results in a larger relative displacement from the center. Thus, as seen in Figure 1, the 202x308 can has the largest ε values for any can associated with error in the radial placement of the thermocouple probe.

The magnitude of ε (Figures 1 and 3) is a result of the fact that shortly after the cans start to heat a gradient in temperature near the center is established for both the radial and axial directions. For the 202x308 can the radial gradient in temperature in the center is greater than that found for the other cans due to a large L/R and small radius. As the can is heated, the temperature gradient around the center and the ε values associated with the thermocouple probe location decrease. The axial effect for the 202x308 can (Figure 3) is very different, because with high θ values the error in axial probe placement is negligible. This indicates that initially, there is virtually no temperature gradient near the can center in the axial direction. As the heating of the can continues, a larger gradient is established and with it larger ε values.

The ε values increase for the axial direction until the temperature gradient near the center starts to decrease with time, after which the ε values decrease with continued heating. Figure 3 also shows that as the L/R ratio decreases (Table 1), the axial heat penetration rate grows in prominence, resulting in larger ε values for low time (see, for example, the 307x306 can). The 603x700 (L/R = 1.13) can seems to be near a transition point (Figure 3) where the prominence of the axial heat penetration rate is evident. The underestimation of α that occurs from errors in thermocouple probe location have associated with it a changing magnitude of precision (C_v) (Figures 2 and 4). Precision in the radial direction for the 202x308 can reached a C_v of 4.0% for low time where the C_v for the 603x700 can never exceeded 0.5%. The axial C_v values generally remain low for all can sizes, the 603x700 being the lowest with the C_v value having a maximum of approximately 0.1%. This indicates that the error in estimated α values due to an error in thermocouple probe location will be minimized by minimizing the relative error of the thermocouple probe location. For the error factor in Table 2 and the can size of Table 1 this would correspond to a relative misplacement error less than 4.0% and not necessarily less than 2.5%. In addition, the L/R value of the can should be such that the heat penetration rates for both axial and radial directions are nearly equal. This can be accomplished using an L/R value in the range of 0.70 to

0.8 .

Error in Can Dimensions

The effect of variation in actual can size on estimating α values were found to be smaller than the effect from variations in thermocouple probe location. This is because the magnitude of can size errors are much smaller than probe position errors (Figures 5,6,7, and 8). Can size variations gave ε values approximately ten times less and C_v values approximately four times less than those found with variations in probe location. Figures 5 and 7 do not indicate any specific kind of trend with θ other than showing that — after long time periods — the error effect of the can dimensions decrease. Error in a can dimension is a factor of the relative change in the can dimension as compared to the overall can size (L/R). For example, the can that showed the largest ε and C_v values for error in the radial can dimension is the 202x308 (large L/R) can and the can that showed the largest ε and C_v values for the axial can dimension is the 307x306 (small L/R). Due to the small magnitude of ε and almost constant C_v values for the θ range, the actual effect of can size variations on calculation of α are miniscule and may be ignored.

Error in Measurement of Time

Time variations result in error effects (Figures 9 and 10) very similar to the error effects of can size, both in magnitude and trend. However, there are decreasing C_v

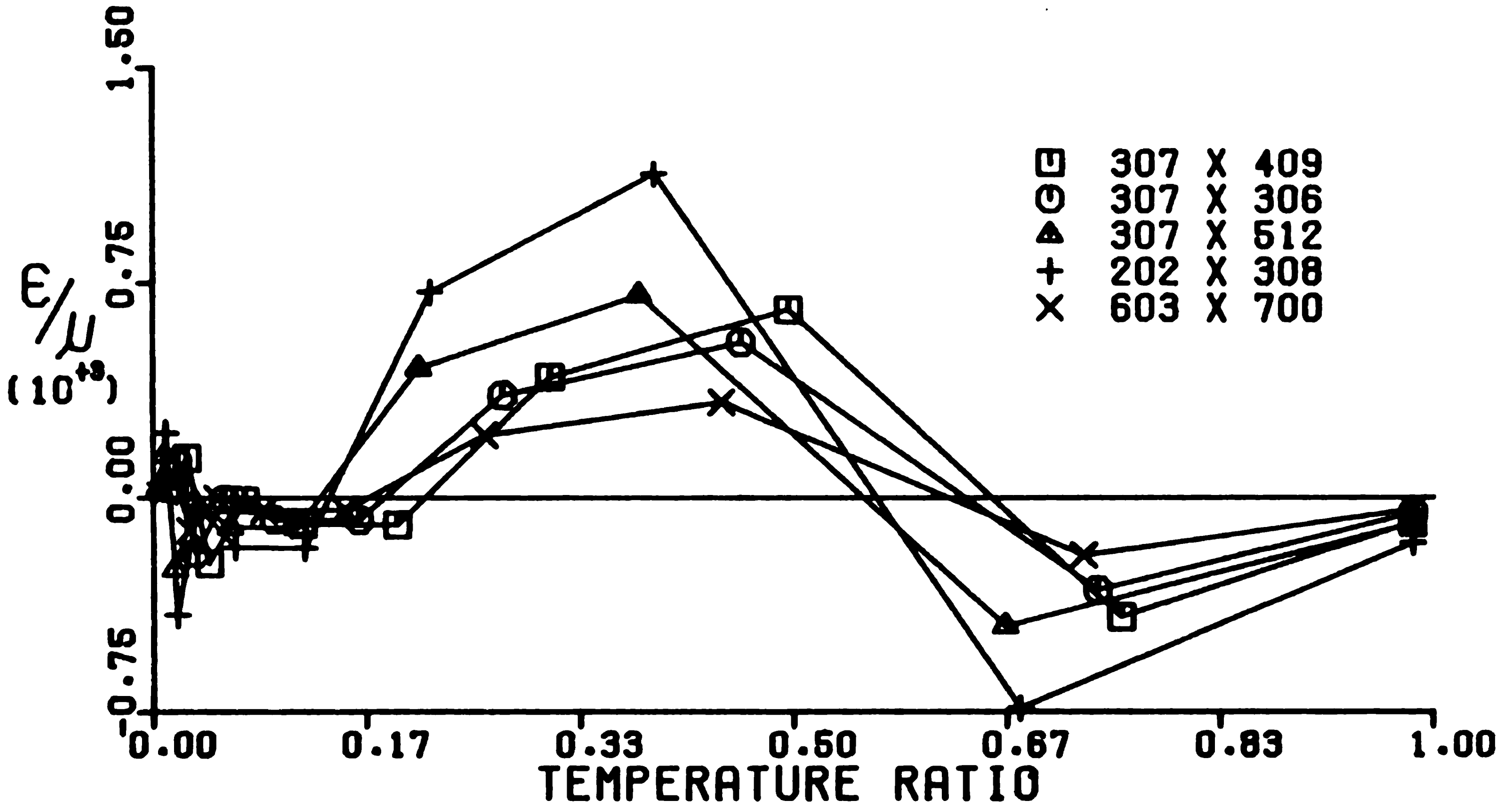

Figure 5. Residual error distribution for error in radial dimension of can.

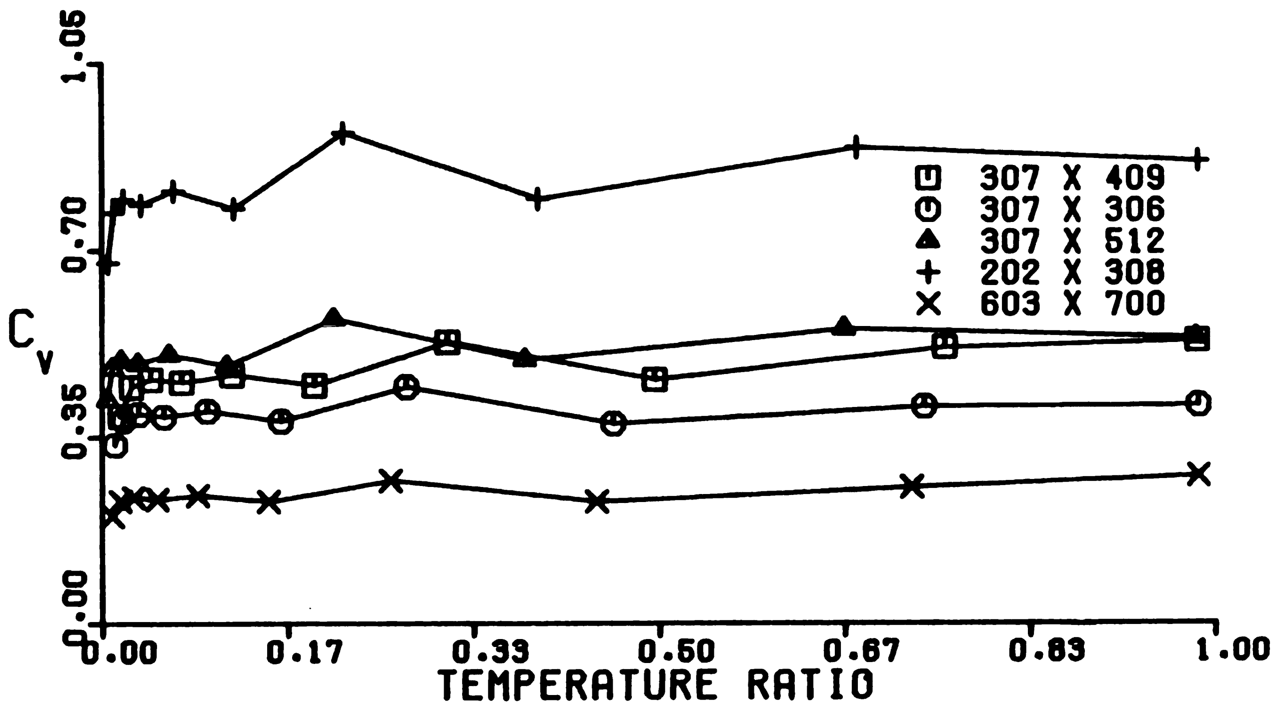

Figure 6. Variance distribution for error in radial dimension of can.

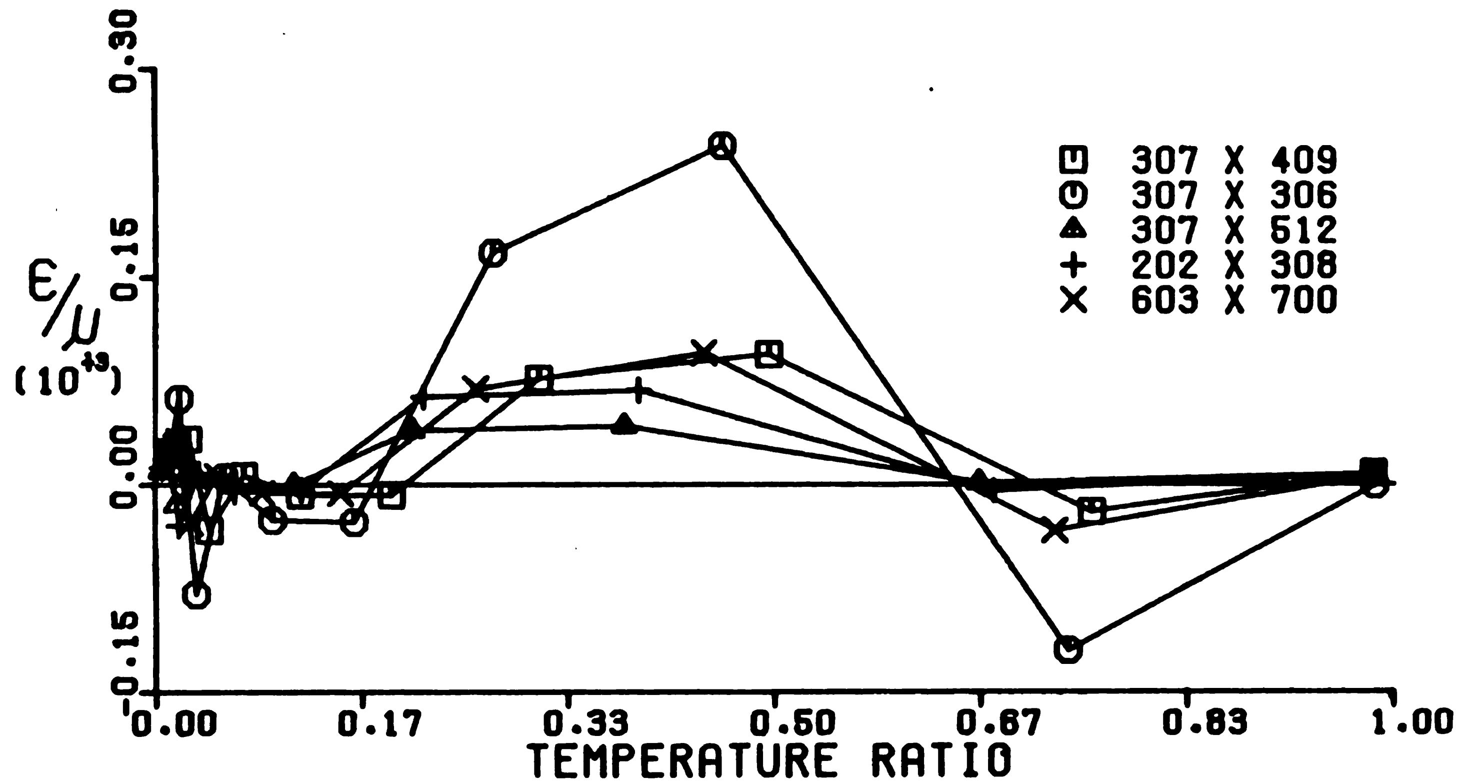

Figure 7. Residual error distribution for error in axial dimension of can.

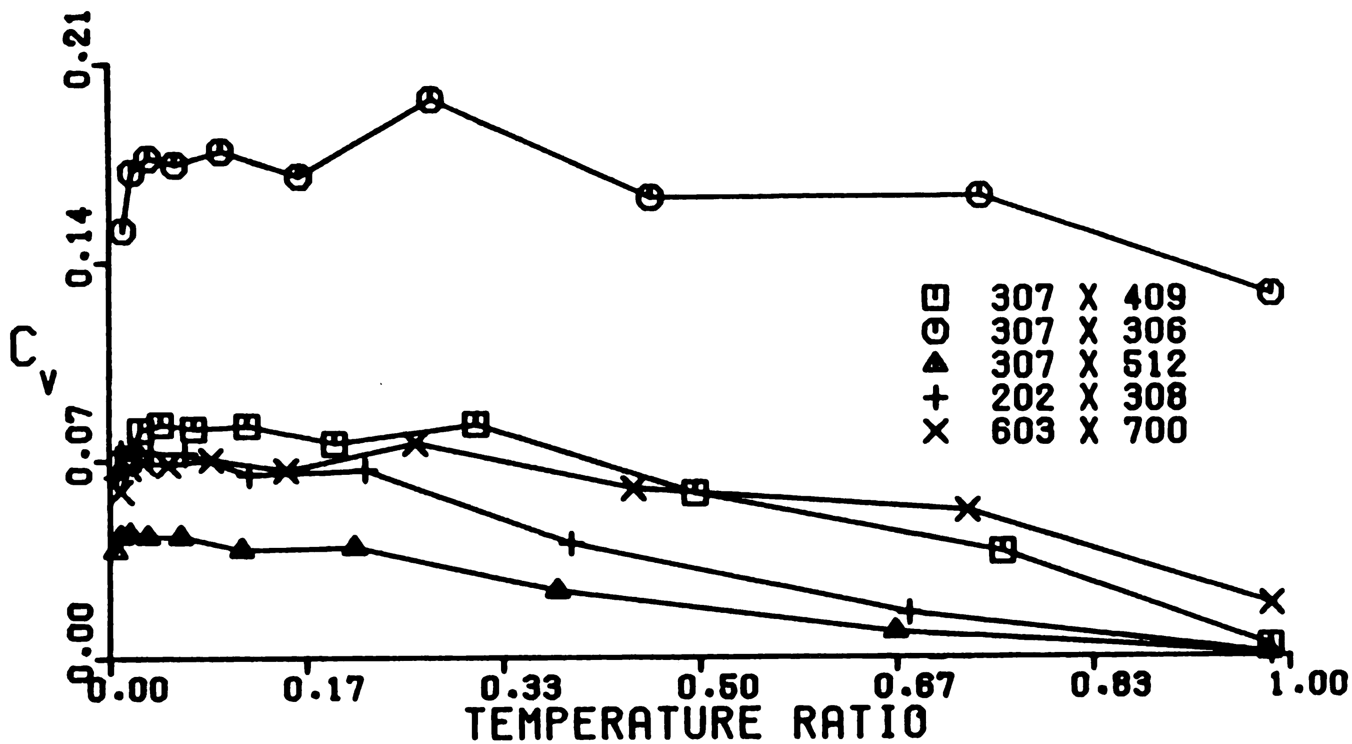

Figure 8. Variance distribution for error in axial dimension of can.

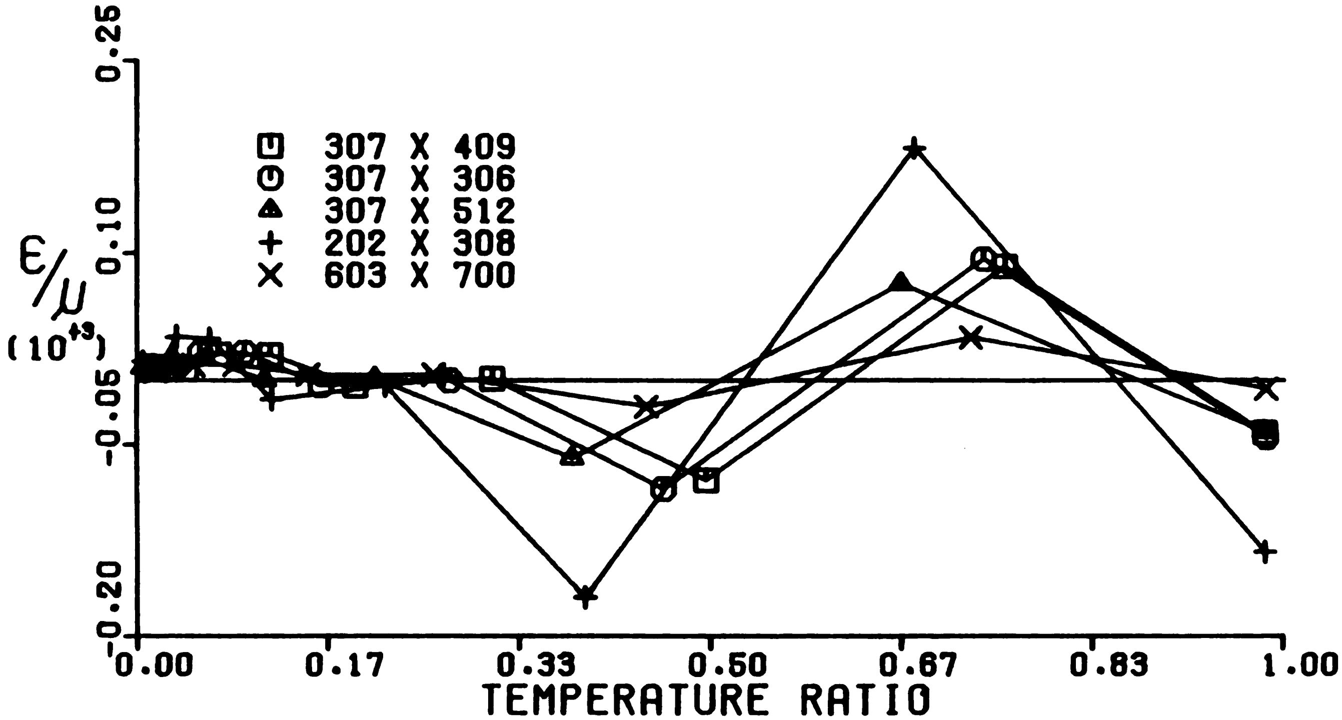

Figure 9. Residual error distribution for autoregressive error in measurement of time.

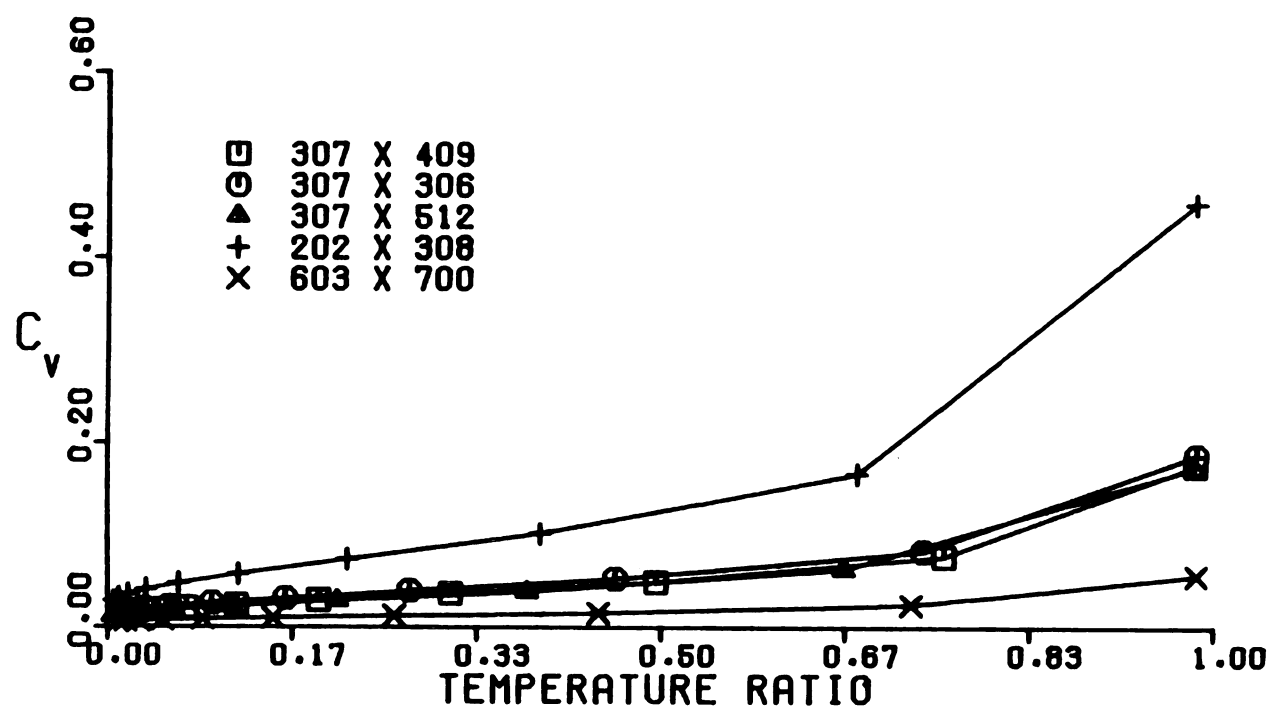

Figure 10. Variance distribution for autoregressive error in measurement of time.

values for decreasing Θ values where there was no trend in C_v for the can size factor. The ε values are the largest for the cans with the fastest heating rate. The indication is that a can that heats slowly will yield a more accurate α value, even though the error in time increases with longer time periods. The high accuracy of the clock used during this study resulted in small values of ε and C_v, which in turn do not cause appreciable changes in the calculation of α. Thus, any error in time measurement may be ignored.

Error in Measurement of Temperature

Temperature variations resulted in the largest errors for any one error factor investigated (Figures 11 and 12). This means that temperature is the most significant parameter in controlling the accuracy of the α estimation. The significance is not only due to the magnitude of C_v and ε but also due to the trends the ε and C_v values display in relation to Θ. The shapes are significant because the curves are identical for the different can sizes (as might be expected from observations of transient heat conduction charts) and because they show a violation of a well-accepted assumption for high and low Θ ranges, i.e., that the errors in temperature measurement do not bias the calculation of α. Figure 11 indicates that the assumption of unbiased α values can only be accepted in the Θ range of approximately 0.90 to 0.05. Outside the range, α values are biased upward for low Θ and downward for high Θ values. Another important point

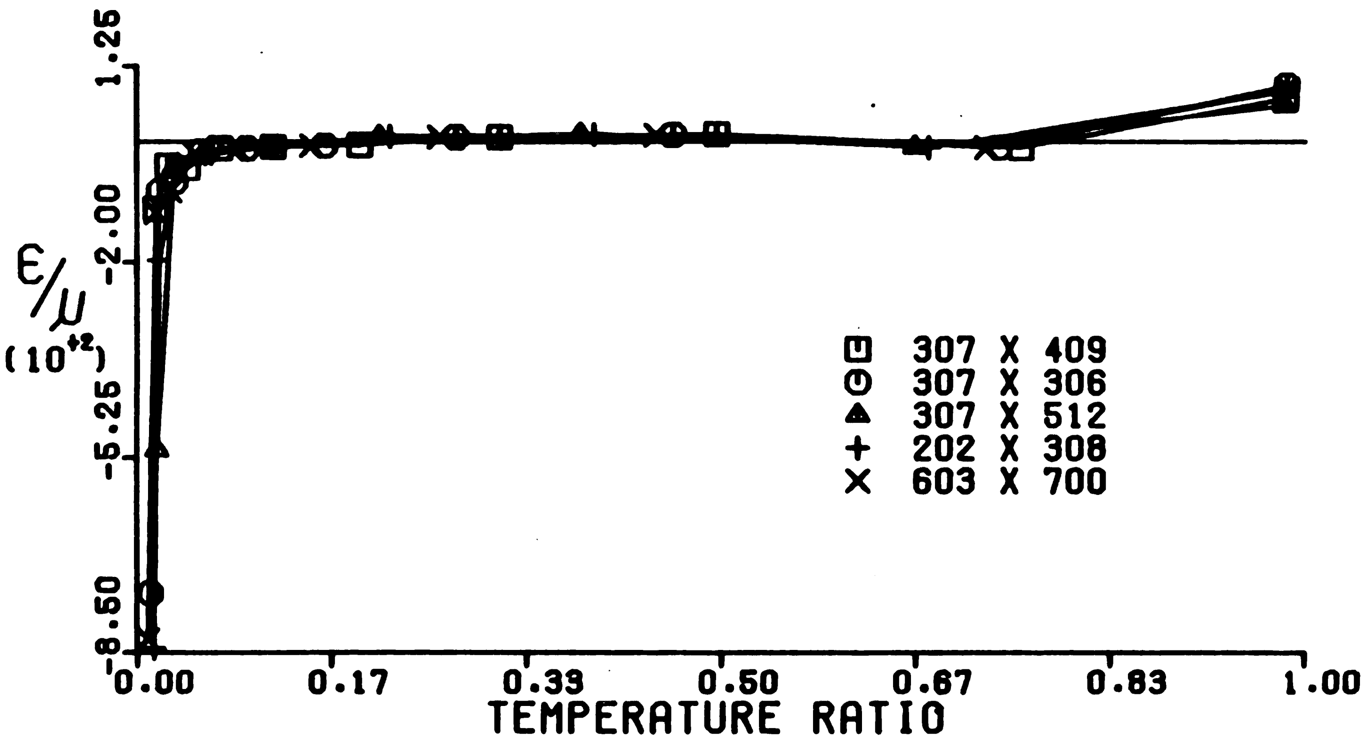

Figure 11. Residual error distribution for error in measurement of temperature.

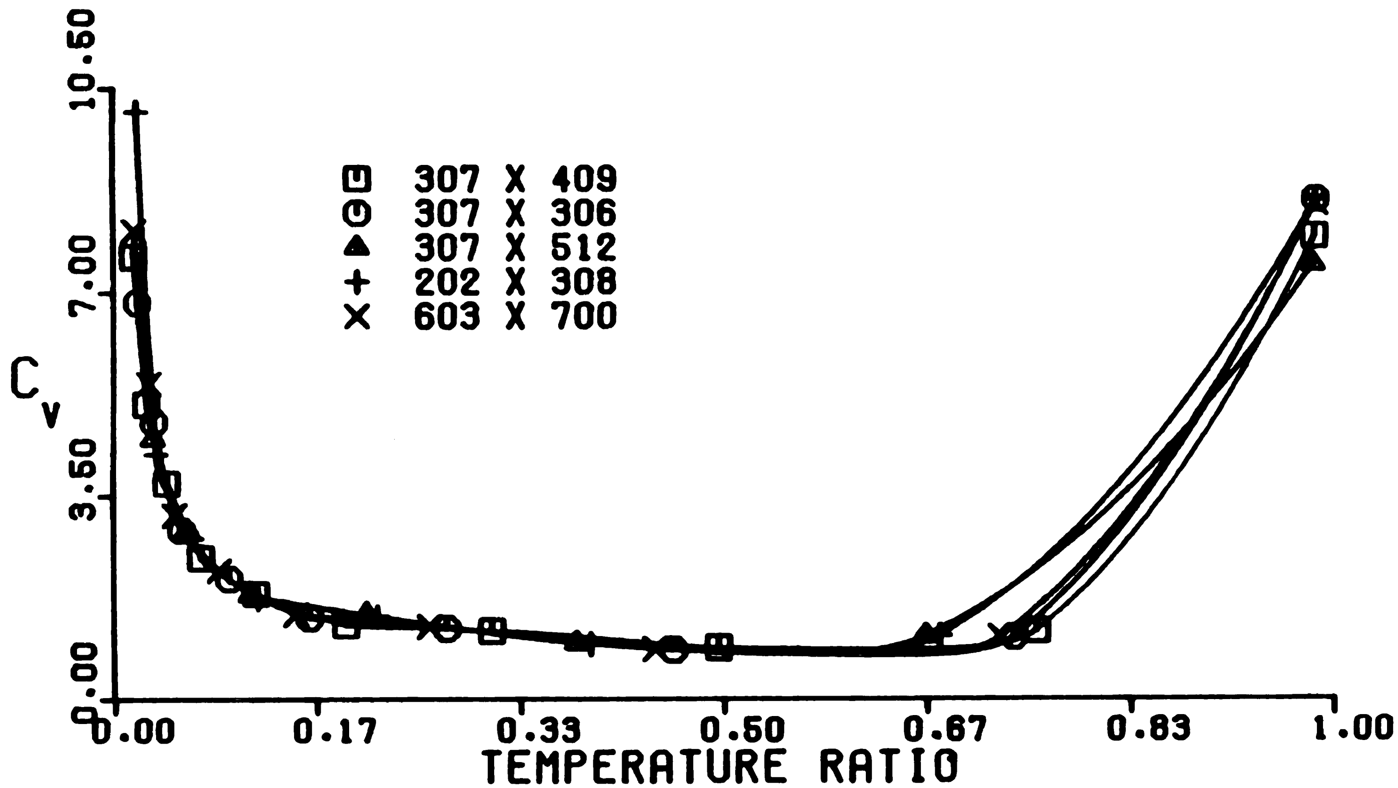

Figure 12. Variance distribution for error in measurement of temperature.

is that an α value calculated strictly with low or high values of θ will not only be inaccurate but will also be less precise due to the increasing values of C_v outside the θ range of 0.85 to 0.15 (Figure 12).

Error of Combined Effect

The influence of temperature on the calculation of α predominates when all the factors listed in Table 2 (except Bi) are varied at once (Figures 13 and 14). When Figures 13 and 11 are compared a drifting upward of ε values is noticed for increased θ when all the error factors are varied. This was not present when only temperature was varied. The upward trend in ε values for Figure 13 is just like that observed for the ε values associated with error in thermocouple probe location (Figure 1 and 3). In this study the more important error in thermocouple probe location is the radial displacement error because all the cans considered have L/R values above 0.8. Therefore, for the sizes and ranges of error factors considered, the predominant error factors in the calculation of α are temperature measurement and radial placement of the thermocouple probe. When only the measurement in temperature was an error factor, a θ range of 0.85 to 0.15 was specified from which an accurate and precise value of α could be calculated; however, with the addition of the thermocouple probe location error, a tighter upper bound on θ might be in order for cans having L/R values different

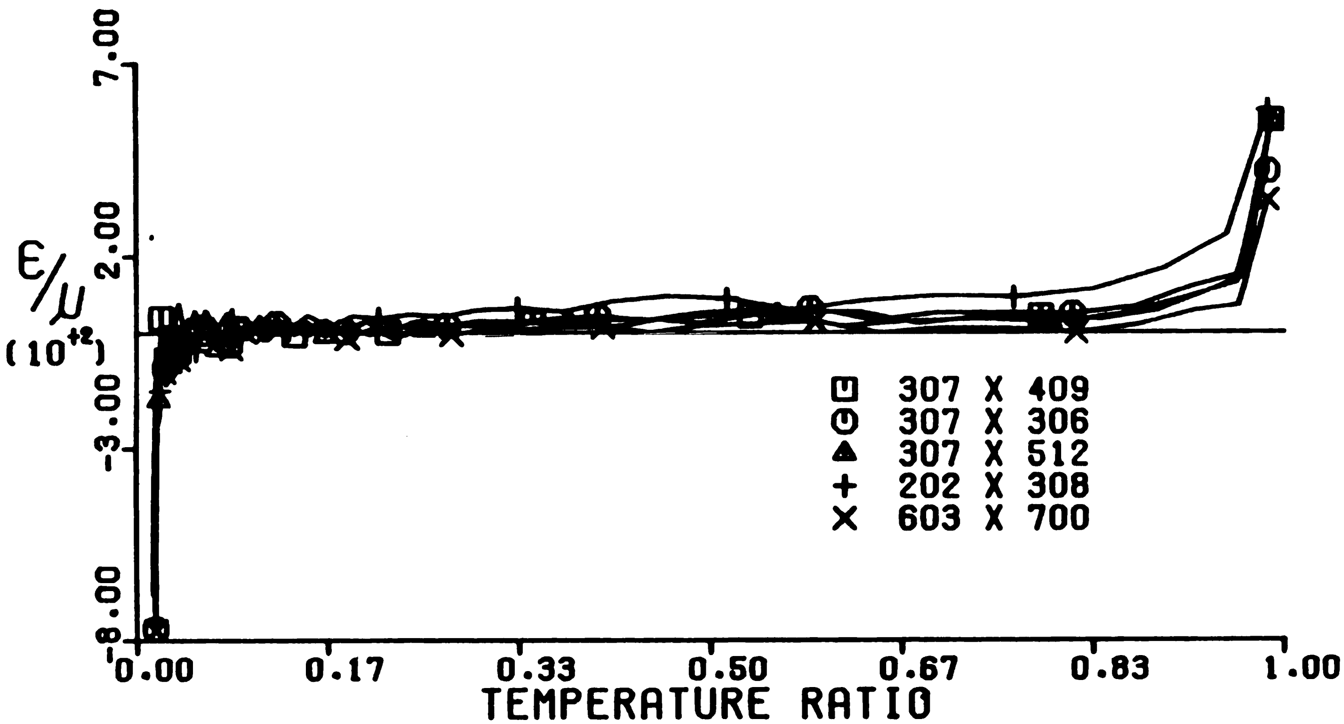

Figure 13. Residual error distribution for combination of error factors investigated by computer simulation.

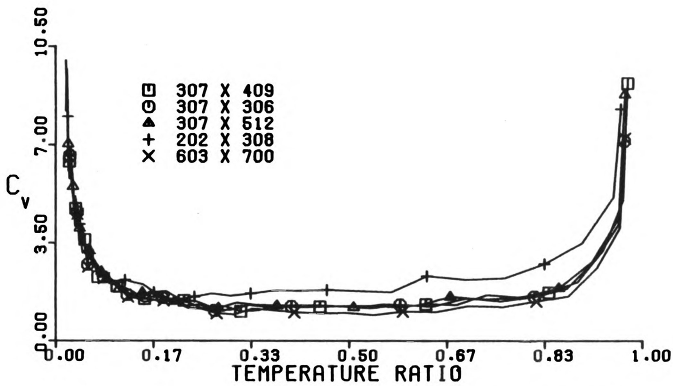

Figure 14. Variance distribution for combination of error factors investigated by computer simulation.

from 0.8.

An L/R ratio of 0.8 is the ratio at which the heat penetration rate for the axial dimension is very similar to that for the radial direction. Therefore, with equal heat penetration rates for the two dimensions, the slope of the temperature gradient around the thermocouple probe is minimized along with any error associated with the position of the thermocouple probe placement. Similarly, Cowell and Evans (1961) observed that when j and f_h are estimated from heat penetration data, the error in the estimates as compared to the asymptote of the heating curve is minimal for L/R ratios of 0.8.

When the temperature difference (ΔT) between the initial product temperature and the medium temperature was varied from 121.1 C to 11.1 C (previously help constant at 56.1 C) the shape of the residual error (ε) and coefficient of variance (C_v) curves remained the same, as found in Figures 13 and 14 discussed above. There was, however, a noticeable difference in the level of the constant C_v region (θ range of 0.15 to 0.85). A coefficient of determination of .9987 was obtained when the mean value of C_v for the θ range of 0.15 to 0.85, was fitted against the inverse of ΔT as

$$C_v = .2677 + \frac{62.21}{\Delta T} \qquad (8)$$

Equation (8) shows that the precision (C_v) associated with estimating α decreases drastically as ΔT decreases below $40.0^{\circ}C$; thus, to obtain an accurate estimate of α the ΔT should remain above $40.0^{\circ}C$.

Error Due to Finite Surface Heat Transfer Coefficients

From the distribution of α in Figures 13 and 14 additional populations of time-temperature points were generated with varying Bi values ($h_t/k = h_s/k = h_b/k$) and compared with time-temperature data calculated assuming 1/Bi = 0.0 (Figure 15). Due to the complexity of trying to analyze the effect of different and varying Bi values for the top, bottom, and side of a can using Monte Carlo simulation, the Biot Number values were assumed to be the same for all the surfaces of the can (taking into consideration the difference in dimension for the radius and length). This assumption was made because the error associated with Bi values is one of assumption (the researcher assumes it is a specific value) or related to a previous measurement of Bi. When Biot Numbers are unknown in calculating α, the product of equations (5) and (7) can be used as the model, because this model allows for estimation of all four of the independent variables (α, h_b/k, h_t/k, h_s/k) using a nonlinear least squares procedure.

From Figure 15 it can be seen that the calculation of α is biased downward when the actual Bi values are not equal to infinity. A 4.0% to 4.5% bias occurs when Bi is actually equal to 50. Even though current literature gives different

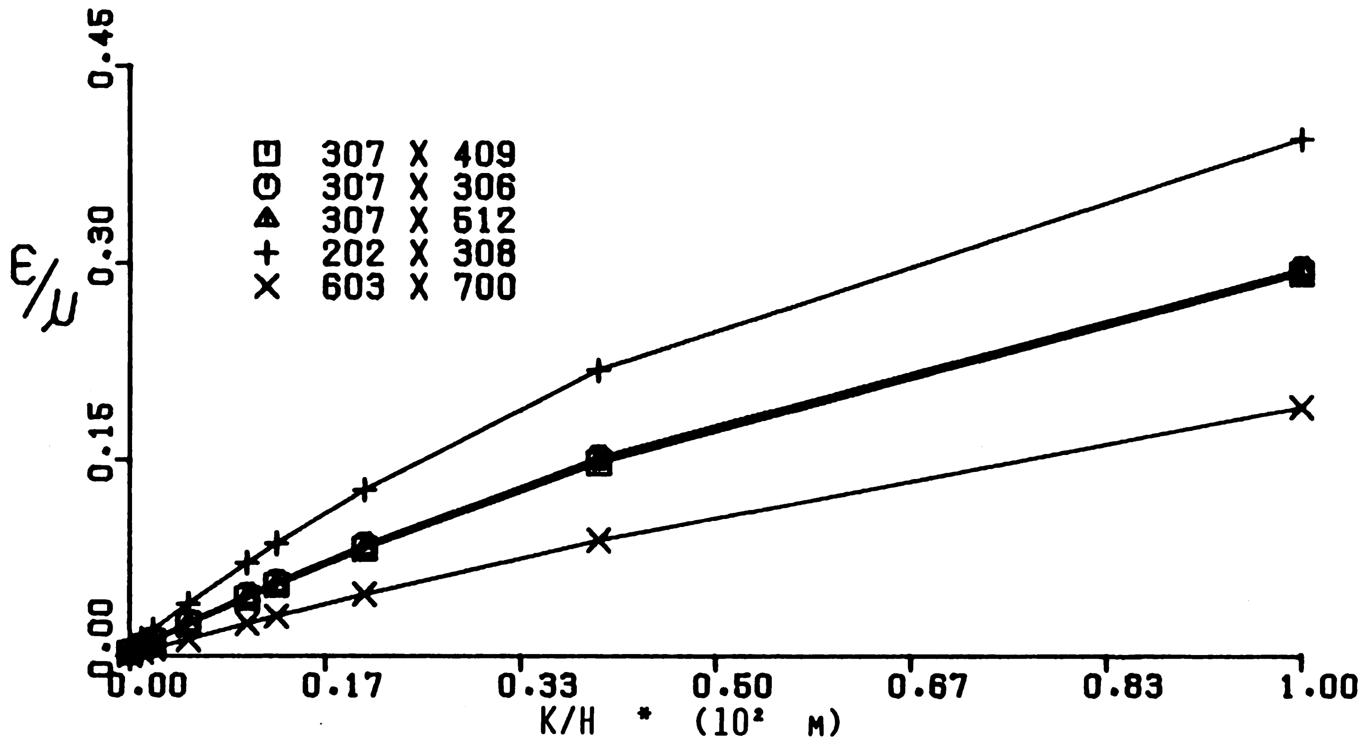

Figure 15. Residual error distribution for error in assumption of Biot Number used in estimation of diffusivity.

values for critical Bi numbers to describe the transition zone for an insignificant surface effect (usually, Bi >40; Heldman and Singh, 1981), a 4.0 to 4.5% error in the calculation of α can be made by neglecting such effects. Similar results were obtained by Gaffney et al. (1980) for the regular regime method. The accuracy in the determination of α values starts to deviate as soon as the Bi values migrate from infinity. The standard deviation of α does not significantly increase (for errors in assumptions in Bi) until Bi is less than 25. Figure 15 indicates that the radius, more so then the length of the can, determines the overall accuracy of the estimated α value.

Since Bi values can affect the precision with which α can be estimated, they should be known or possibly estimated simultaneously with α. When Bi is greater than 200, it has little effect on the estimation of α (Figure 15) and because of this, it is very difficult to estimate. Note, a 2-3% variation in α would cause an estimate of Bi to vary from infinity to 100 (Figure 15; Ramaswamy et al., 1983). In addition, sensitivity analysis shows that α and the surface heat transfer coefficients are strongly correlated. Uno and Hayakawa (1980a) advocated simultaneous estimation of α, Bi_s, Bi_b, and Bi_t from heat penetration data. Their results showed that errors on the order of 26 to 200% were possible for the Bi values when considering error in parameters similar to those in Table 1.

Sensitivity Coefficient Analysis

Sensitivity coefficients (equation 9; Beck and Arnold, 1977) are calculated by taking the first derivative of the model $\theta(\alpha,Bi)$ with respect to each of the independent variables (α,Bi).

$$\text{sensitivity coefficient ratio} = \frac{\alpha \dfrac{d\theta}{d\alpha}}{\left(\alpha \dfrac{d\theta}{d\alpha}\right)_{max}} \qquad (9)$$

Sensitivity coefficients (SR) indicate the change in the response, in this case the temperature ratio, as a function of the variable. There are two important qualities of the model that can be learned from the sensitivity coefficients. The first is the correlation that the independent variables may have with each other, which is important when attempting to estimate them simultaneously. The second quality learned has to do with the magnitude of the sensitivity coefficient with respect to the response. Larger sensitivity coefficients areas are areas where small changes in the response cause large changes in the independent variable, making it easier to obtain precise estimates of the independent variables. In conjunction with this last quality are the relative magnitudes that different sensitivity coefficients have with each other. The parameter with the larger sensitivity coefficients will be the parameter that is estimated more precisely from the nonlinear regression analysis.

Figures 16 through 19 are plots of the sensitivity coefficient ratio (SR) for each of the independent variables, where the denominator of the ratio is the maximum sensitivity coefficient value. SR values ranges from 0.0 to 1.0. Plots were made for three different can sizes, 307x300, 307x409, and 401x410 (L/R = .873, 1.327, 1.138 respectively) and for dimensional surface heat transfer coefficients (h/k) of 200, 1100, and 120000 m^{-1}, for the top, bottom, and side surface heat transfer coefficient (a total of 54 plots). The h/k values listed above correspond to Bi values of 8-11, 45-60, and 5000-6200 for the different can sizes. The first and last Bi values are at the two extremes of importance (very significant and negligible) with regard to the model, and the middle Bi value corresponds to the transition zone of importance. The can sizes represent two cans with the same radius and different length and two cans with similar length and different radius. The L/R ratio range is similar to those described in Table 1.

It was observed that having h/k values equal to 120000 m^{-1} resulted in the SR value of h/k being strongly correlated with the SR of α (Figure 16). In addition, the magnitude of the SR value of α was 3500 to 1 of the SR value of h/k (when equal to 120000 m^{-1}) indicating that any attempt to simultaneously estimate α and the corresponding h/k value would result in potentially erroneous values.

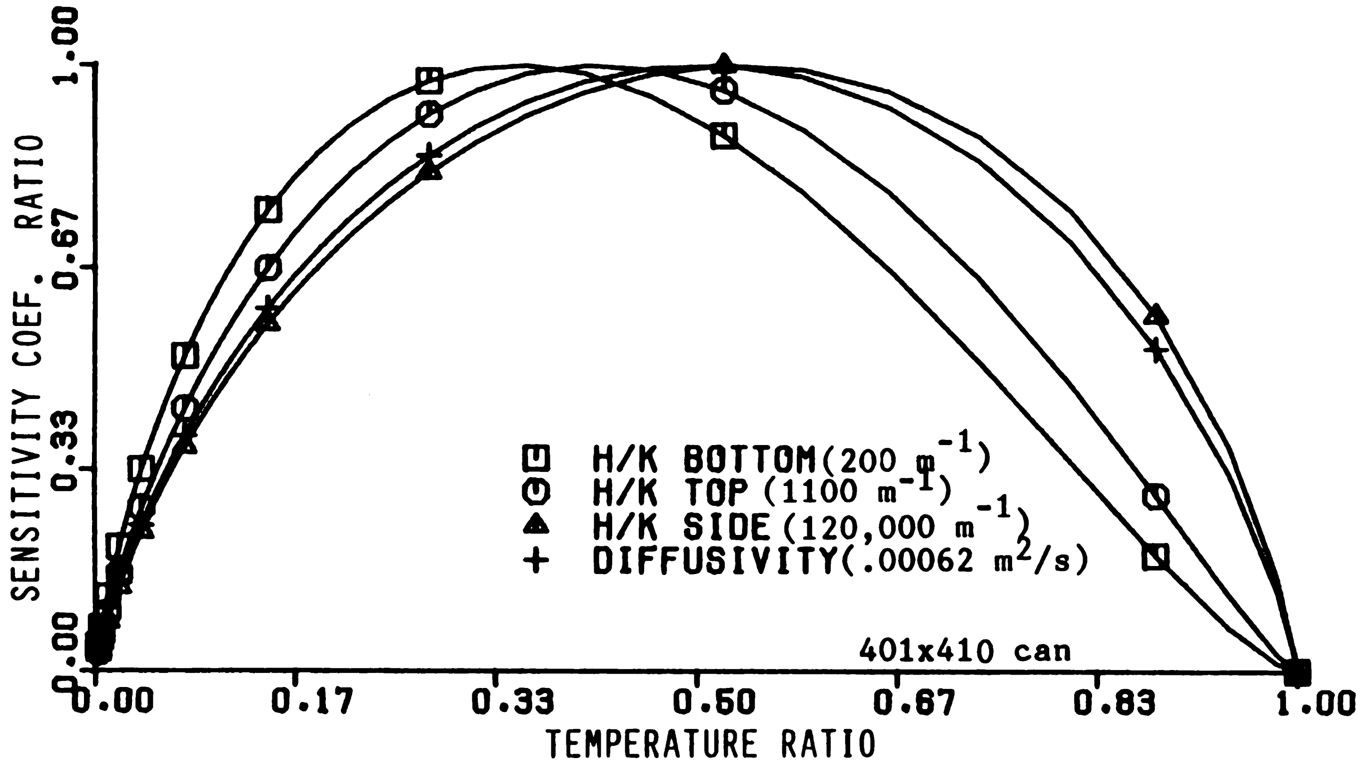

Figure 16. Sensitivity coefficient ratio as a function of temperature ratio for top (h_t), bottom (h_b), and side (h_s) surface heat transfer coefficients and for diffusivity, all being simultaneously estimated from thermal process data.

This was not unexpected considering the above discussion for Bi values greater than 200. The plots also show that h_s is always correlated with α. This means that it is not advisable to simultaneously estimate α along with three separate surface heat transfer coefficients. This is further verified by the fact that even when h/k is equal to 200 m^{-1}, the SR for h/k is 60 times smaller than that for α. If α were known and the three different surface heat transfer coefficients were being simultaneously estimated, it would depend on the relative magnitudes of the h values as to whether or not the values could be estimated accurately.

The largest separation of the SR values occured when the bottom, top, and side h/k values were respectively 200, 1100, and 120000 m^{-1} (Figure 16). Only when the three coefficients are very different from each other can they be separately estimated with accuracy. When the three surface heat transfer coefficients were lumped together so the surface heat transfer coefficient was assumed equal for all sides of the can, the SR plots showed more variation with regard to the dimensions of the can than did the analysis of the three separate h/k values (Figures 17,18,19). Conversely, the lumped analysis of h/k showed little if any shape variation in SR with respect to the size of h/k. However, the magnitude of the SR values was the same for both cases. This indicates that it is not advisable to estimate α and a lumped h/k value simultaneously.

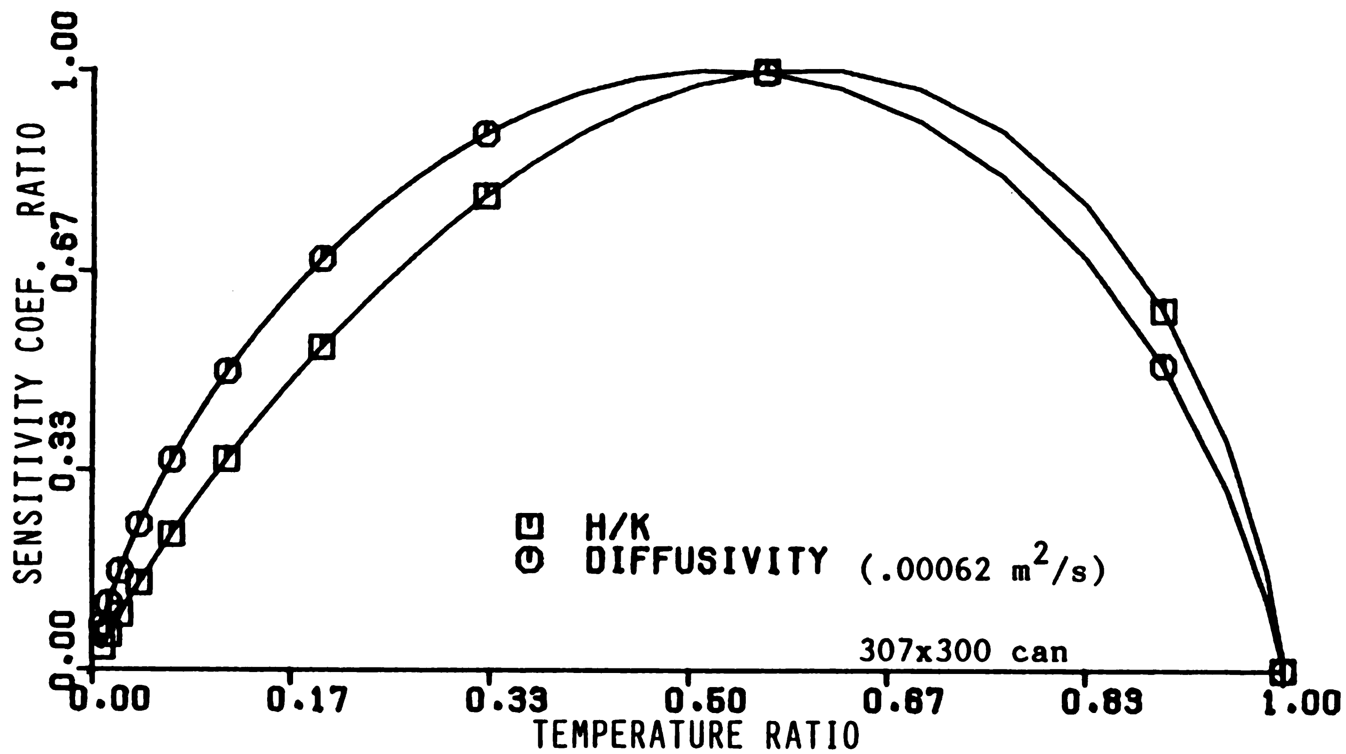

Figure 17. Sensitivity coefficient ratio as a function of temperature ratio for diffusivity and an overall surface heat transfer coefficient, estimated simultaneously from thermal process data from a 307x300 can.

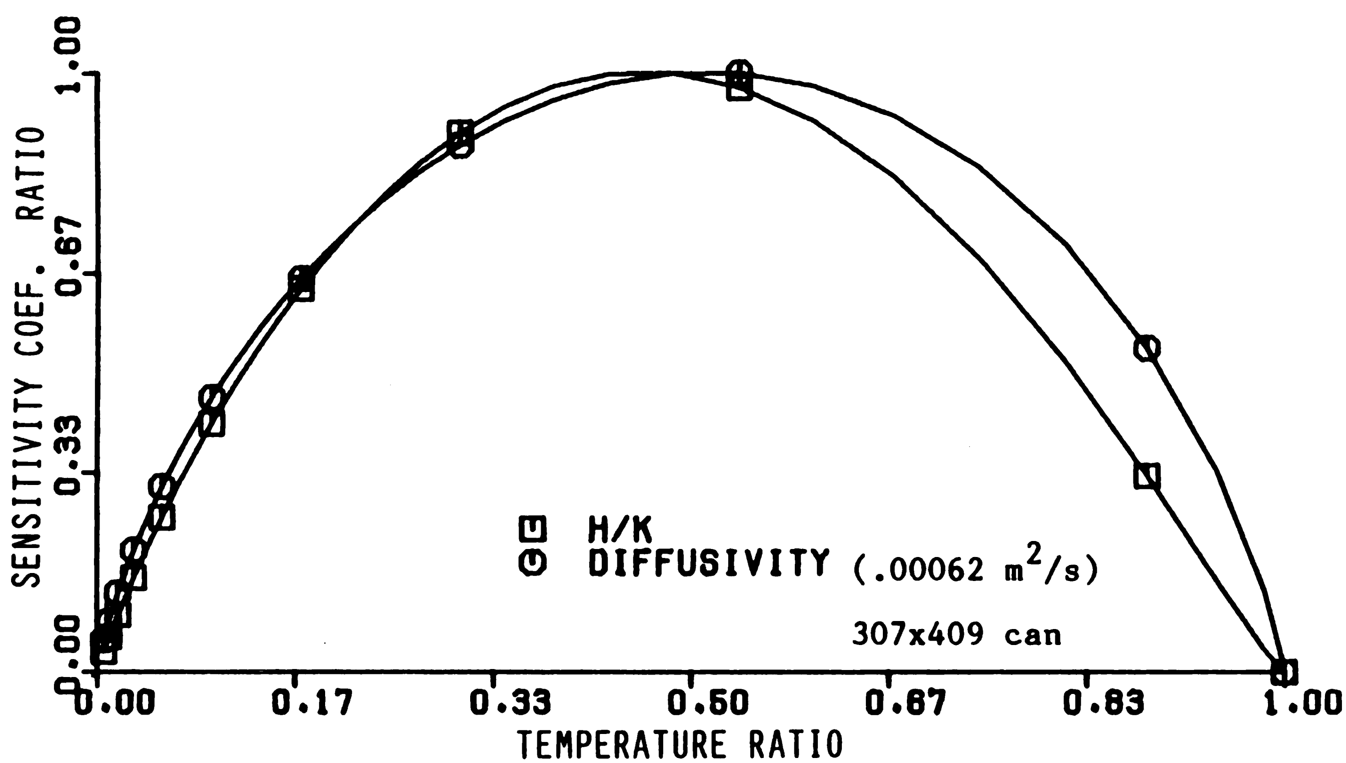

Figure 18. Sensitivity coefficient ratio as a function of temperature ratio for diffusivity and an overall surface heat transfer coefficient, estimated simultaneously from thermal process data from a 307x409 can.

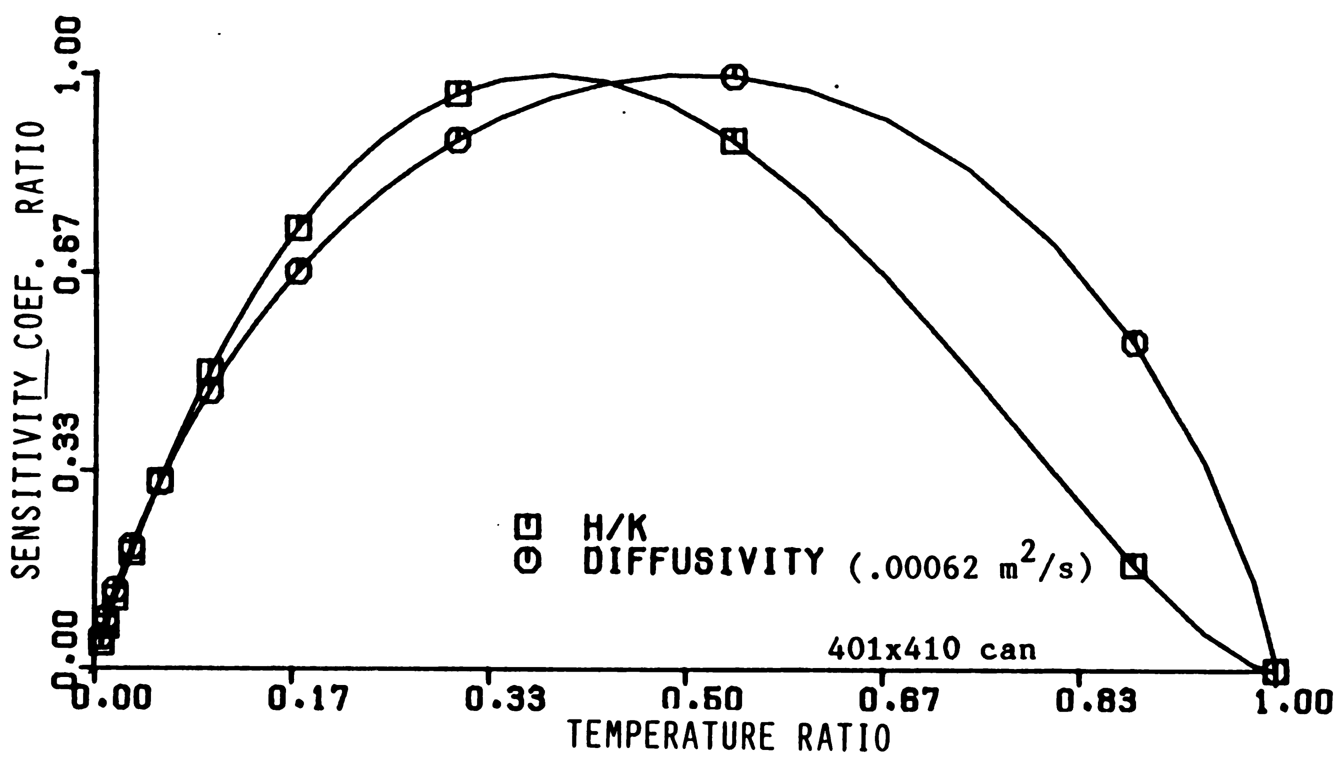

Figure 19. Sensitivity coefficient ratio as a function of temperature ratio for diffusivity and an overall surface heat transfer coefficient, estimated simultaneously from thermal process data from a 401x410 can.

One last thing that can be observed from the sensitivity coefficient plots is that the SR values are the largest in the center of the θ range. This is in agreement with Figures 13 and 14 because the θ range of 0.15 to 0.85 promotes precise estimates of α. With larger SR values more precise estimates can be made.

Error Effects on Regular Regime Method

From the same population of time-temperature points, with varying Bi values, a potential error of 4.0% in α can be obtained in the calculation of α from f_h. This occurs using the Olson and Jackson (1942) equation (10), where Bi was equal to 50 but assumed infinite. The equation may be written as

$$f_h = \frac{1}{\alpha} * \frac{.398}{\left[\dfrac{1}{R^2} + \dfrac{.4267}{L^2}\right]} \tag{10}$$

The α value calculated from the analytical model always resulted in an underestimation of α, whereas the Olson Jackson equation first overestimated the actual α value and then underestimated α as Bi values decreased. In Figure 13 it can be seen that the α values start to be biased upward as the θ values decrease. This causes the α value, calculated from the Olson and Jackson equation, to be overestimated because the slope of the heating curve is increased due to the increasing upward bias of α and because the calculation of α from the analytical model places more importance on the intermediate values of θ.

The overestimation of α (α_2) from f_h for the different can sizes (Bi = ∞, is data set 1) does not follow the same trend as that found for the underestimation of α (α_1) from the analytical model (Table 3). The value of α calculated from the analytical model for the 603x700 can was very accurate and a similar accuracy was expected for the α value calculated from the f_h values. In turn, the 307x409 can gave the most accurate value of α calculated from f_h, with the value of α from f_h for the 603x700 can having a lower accuracy.

To determine if the above trend was due to the errors associated with the data of first term approximation, a population of 100 points with a constant C_v (1.0%) for α, was generated and called data set 2. The f_h and α were calculated for each can size (Table 3) from this population of points. The same trend in can size was noticed in both the α values calculated from f_h for the data set 1 and data set 2 (Table 3). From the similarity in trends of the two calculated α values it appears that the effect of the error terms in Table 2 on α is one of a linear (upward bias) shift in α and that the variation in error associated with specific can dimensions is mainly due to the first term approximation (i.e., regular regime) method.

Table 3

Summary of α and f_h values obtained from different data sets containing different error distributions (1 - error distribution of figures 13 and 14, 2 - constant C_v (1.0%) of α).

Can Size	α of Data Set 1 α_1 ($m^2/hr \times 10^{-3}$)	α from f_h Data Set 1 α_2 ($m^2/hr \times 10^{-3}$)	α from f_h Data Set 1 α_3 ($m^2/hr \times 10^{-3}$)
307x409	.618	.621	.599
307x306	.618	.627	.613
307x512	.619	.624	.603
202x308	.616	.624	.605
603x700	.620	.625	.606

Actual α = .620 x 10^{-3} m^2/hr

Figure 20 presents the first term approximation error ((approximation - actual)*100/(actual)) in the calculation of θ values for all five can sizes. As the L/R ratio increases, the error in the first term approximation increases. A L/R ratio of about 0.94 represents a can size where the error of first term approximation associated with the radial direction is the same as that found in the axial direction. This explains why the 307x306 can displays an α value closest to the actual (Data set 2, Table 3). This also explains why the error (except 307x409 can) in α calculated from f_h increases as the L/R increases. However, it is not known, without further investigation, why the

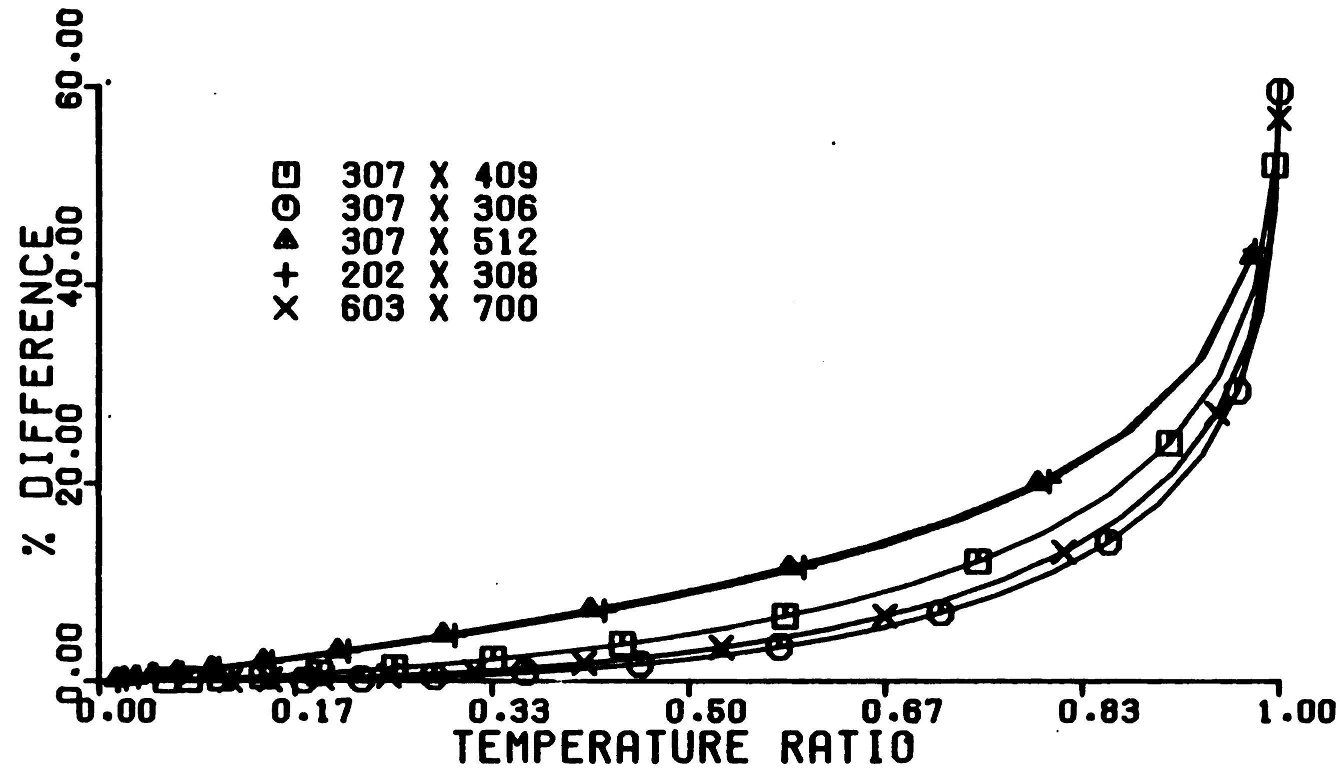

Figure 20. Percent difference of the temperature ratio for the first term approximation and infinite series solution.

307x409 can size deviates from the expected L/R ratio trend.

With the addition of the error factors listed in Table 2 the calculated α values from f_h become close to the actual α value. This is an apparent accuracy because it was assumed that heating follows Fourier's heat conduction equation; hence, the prediction of α calculated from f_h should follow the α values found using data set 2 instead of the apparently accurate α values calculated from data set 1. There is about a 3.5% change in the calculated α when the error factors in Table 2 are included in the calculations of α from f_h. If the errors in Table 1 change, it becomes very difficult to make any judgment regarding how they will influence the estimation of α calculated from f_h, because the estimated α values will fluctuate around the α values found from data set 2.

Summary and Conclusions of Theoretical Develomment

A well-conditioned model is one that performs as expected for a specific range of errors in the input parameters. With the original assumptions given at the beginning of this chapter it was expected that the analytical solution to Fourier's heat conduction equation would yield a well-conditioned model to be used to accurately estimate the thermal parameters (α, and h_i; where $i = t,s,b$) of a thermal process. The condition of the analytical model was, when α was calculated from data ($h_i = \infty$) containing errors (Table 2), largely dependent on the errors associated with temperature measurement and to a lesser extent dependent on the errors in thermocouple probe location. Errors in can dimensions and time measurement had minor influence on the prediction of α because of the magnitude of the error of the respective parameters.

If there were only errors of can dimensions and time in a process, they would indicate that a slowly heated can (large can) with a L/R ratio of about 0.8 should be used to increase the accuracy of the estimation of α (Figures 5,7, and 9). This same trend was noted for errors in thermocouple probe location (Figures 1 and 3). Therefore, any actions taken to minimize the effect of error in thermocouple probe location would also minimize the effect of error occurring due to can dimensions and time measurement. For errors in thermocouple probe location, the size of the can was more important in lowering the error associated with the estimation of α than the L/R ratio.

Can size was not a factor in influencing the condition of the model when only errors in temperature existed. For temperature errors, the accuracy in predicting α ($h_i = \infty$) was increased if the temperature data used was limited to a θ range of 0.85 to 0.15 (Figure 1). This criterion for θ predominates when all the error factors mentioned above are present and is supported with the sensitivity coefficient analysis of the model (Figures 13 and 16). The thermocouple probe location error is also noticeable when all the errors (Table 2) are present, causing a tighter upper bound on the θ as the can size decreases. In addition, when the Biot Number is assumed infinite but is actually lower than 200, the model underestimates α by a value over 1.0% (Figure 15).

Strong correlations exist with the sensitivity coefficient ratios (SR) of α and h_i/k (where i = t,s,b); thus, any attempt to simultaneously estimate α along with the surface heat transfer coefficients may result in erroneous values. Only when the surface heat transfer coefficients (h_i; i = t,s,b) are very different from each other are their values uncorrelated (Figure 16). Even when just an overall surface heat transfer coefficient (h/k) is to be estimated simultaneously with α, the precision of the estimated h/k would be low, due to the magnitude of difference between the SR values of α and h/k (60 to 1). When estimating h/k from thermal process data, a product with a known α should be used in addition to having a Bi less than 40.

When the regular regime (first term approximation) method was used in estimating α, large fluctuating α values ($h_i = \infty$) resulted for different can sizes. The fluctuations occurred because of the reliance of equation (10) on the low, biased, and highly variable θ values.

When a nonlinear least squares method is used to estimate thermal parameters from Fourier's heat conduction equation, in conjunction with the error factors investigated in this chapter, the following procedures should be used to insure an accurate and precise estimation of α.

1) Use a can that allows for the relative misplacement of the thermocouple probe to be less than 4.0%. For errors consistent with those in Table 2 a 401x411 (No. 2 1/2) or larger can would be adequate.
2) Use a can with a L/R ratio close to 0.8 to minimize the influence of can dimension and time measurement errors, and to some extent thermocouple probe placement errors.
3) Determine the magnitude of the surface heat transfer coefficients in the thermal process using a product with known thermal properties that allows (Bi less than 40) for its estimation.

If Bi is greater than 200 it can be assumed infinite.

4) Limit the range of data used in calculating thermal diffusivity to temperature ratio (θ) values between 0.15 and 0.85 (For errors consistent with those in Table 2).

5) The temperature difference between the initial product temperature and the heating medium temperature should not be lower than 40.0° C (For errors consistent with those in Table 2).

Chapter II

Experimental Analysis

Introduction

When experimentally obtaining thermal process data there are a number of factors that become incorporated into the results and, thus, affect the "true" values. Chapter I reviewed a number of these factors (position of thermocouple probe, can dimensions, measurement of time and temperature, and assumptions concerning the surface heat transfer coefficient) and, using computer simulation, elucidated their effects. However, there are a number of other factors that are best investigated from actual thermal process data.

One of these factors is heat conduction down the thermocouple probe, because this phenomenon is very difficult to mathematically evaluate. The main reason is that analytical solutions for heat conduction through a thermocouple probe only exist for special configurations, and with the small size of the probe, finite difference and finite element solutions require an extensive grid structure and computation time. The thermocouple probe can cause a significant error in time-temperature data because it usually has a higher thermal conductivity than the thermal conductivity of food. This results in the probe tip being partially heated by the probe itself. The thermocouple acts very much like a pin fin on a heat exchanger.

Other important factors that require experimental investigation are, come-up time, filling (i.e., head space and air inclusions), pretreatment (i.e., blanching and exhausting), and food product homogeneity. Usually these effects can be eliminated through the experimental design; however, these and many other factors, like those discussed in Chapter I, will show themselves in the overall precision of the data. An additional factor that will should be considered in the overall precision of the data collected is that of biological variation in the food items.

This chapter deals with methods of compensating for heat conduction down the thermocouple probe, combined with quantifying the precision associated with the experimental procedure of estimating thermal diffusivity from thermal process data using a model food system. The precision of the procedural method will then be used to evaluate any biological variations that may be present in a food item. It will also be used to verify the thermal diffusivity estimation procedure.

Literature Review

Thermocouple Probe Error

Any measurement of temperature — using a probe — can be biased due to heat conduction along the probe and to displacement of material to accomodate the probe (Ecklund, 1955; Jaeger, 1955; Cowell et al., 1959; Burnett, 1961; Beck, 1962; Beverloo and Weldring, 1969; Jen and Li, 1974; Chen and Danh, 1976; Chen and Li, 1977; Yoshide et al., 1982). Differences in the thermal properties of the probe and the material being measured accentuate this bias. When using thermocouples to measure the temperature of food systems just such a difference in thermal properties exist: approximately a 130 to 1 difference in α and 110 to 1 difference in k. Bias can be eliminated when measuring the temperature of a steady-state system by bringing the leads of the thermocouple through a significantly long zone of constant temperature. This minimizes any temperature gradients that may occur between the probe and the material.

Equilibrating the temperature of the probe by bringing it through a constant temperature zone, can be used in transient heat conduction problems by having the probe go through a significantly long axis of symmetry (Dickerson, 1966; Gaffney et al., 1980). Dickerson (1966) points out that, for a thermocouple mounted (axially) in the geometric center of a cylinder 5.46 cm in diameter and 22.86 cm in length, the thermocouple passes through approximately 8.9 cms of length where the temperature gradient is only normal to the probe. This length is sufficiently long to eliminate, near the tip, any temperature gradients found along the probe. Likewise, Gaffney et al. (1980), using a 1.63 cm diameter and 7.62 length tube showed that by mounting a thermocouple through the axis of the cylinder, the errors associated with heat conduction along the thermocouple would be eliminated. The L/R ratio of these cylinders are both greater than 4.0. The L/R ratio for a conventional can will rarely exceed 1.7 and, thus, will have few, if any, constant temperature gradient zones.

The mounting of thermocouples for thermal processing tests are typically done radially and result in bias data. It is interesting to note that, even though the measurement of temperature using radially mounted thermocouples is in error, there have only been three detailed studies as to the magnitude of this error (Ecklund, 1955; Cowell et al., 1959; Beverloo and Weldring, 1969). The main reason for neglecting heat conduction down the thermocouple wire is the use of the regular regime method of estimating α. Ecklund (1955) demonstrated that the slope (f_h) of the heating curve did not change when "nonprojecting" (Ecklund, 1949) thermocouples were used as compared to surface mounted thermocouples. Ecklund (1955) did show, however, that the lag phase (i.e., the intercept (j) of the heating curve) decreased significantly with the use of the "nonprojecting" thermocouple. To compensate for the decrease lag phase, Ecklund proposed the use of "corrected" j values, which were calculated from an empirical table of correction factors. Gaffney et al. (1980) substantiated Ecklund's (1955) results with the use of axially and radially mounted thermocouple probes in a long cylinder where f_h was the same for both probes. Therefore, when using the regular regime method for estimating α from thermal process data, errors associated with heat conduction down the thermocouple probe can usually be ignored. Since the temperature matching method uses the whole heating curve when estimating α, any error that occurs in the measurement of temperature will affect the results.

The effect the thermocouple probe has on the slope (f_h) of the heating curve and thus α, is to some extent dependent on the size of the thermocouple wire. Cowell et al. (1959) indicate that when the wire becomes large — compared to the size of the can — changes in the f_h values can occur. For the typical can size, the Ecklund probe will not affect the f_h value.

The magnitude of the error in temperature measurement increases rapidly from time zero and reaches a maximum shortly afterwards; it then decreases asymptotically to zero at long time (Jaeger, 1955; Cowell et al., 1959; Beverloo and Weldring, 1969). Beverloo and Weldring (1969) showed that error in measurement is directly proportional to the rate of temperature change with time, and that both follow a parabola. Jaeger (1955) presents an analytical solution for the temperature of a solid wire normally transversing an infinite slab, with the wire having high thermal conductance and the slab having low conductance. The solution can be used to estimate the error associated with axially mounted thermocouples. Cowell et al. (1959) used Jaeger's (1955) solution to investigate data collected from a 5 by 5 cm cylinder. The results followed the same trend that Jaeger's (1955) analytical solution predicted, but were consistently lower than the predicted values. The discrepancy was thought to result from the surface heat transfer coefficient between the wire and the heating media being less than infinity - as assumed. Beverloo and Weldring (1969) have found that, when considering thermocouple assemblies (e.g., Ecklund thermocouples), the error in the measurement of temperature is characteristic of the size and material used for their construction. Hence, it is difficult to predict errors in temperature measurements from analytical solutions which assume that the shape of the thermocouple is a long wire made of a single component.

Beverloo and Weldring's 1969 paper is of special interest, not only because it characterized the error associated with heat conduction along the thermocouple, but also because they measured the error effect of 16 different thermocouples that were mounted radially in a cylinder. The thermocouples studied varied greatly in shape and construction. On the average, the error in temperature measurement was dependent on the wire thickness and the diameter of the probe. These errors ranged from 0.3 to 23.0% of the temperature difference between the initial temperature and that of the heating media for a 10cm by 50cm test cylinder. In thermal process data this error would correspond to errors of 0.2 to 13.0 deg C. Two of the thermocouples measured were the same as those used in this research, i.e., a "nonprojecting" Ecklund thermocouple and a mineral insulated thermocouple. Both were found to have relative errors in temperature measurement of about 3.0%.

Model Food Systems

In considering thermal process data, a product with known thermal properties must be used to quantify the following: 1) the effect of heat conduction along the thermocouple probe, 2) the error associated with neglecting finite surface heat transfer coefficients, and 3) the effect of inherent process variations on the estimation of α. The thermal properties of water are well documented and, thus, any product that has a very low solids content can be used as a model food system. To use water, convection inhibitors need to be added. A number of inhibitors have been used in published literature (Cowell et al., 1959 — 5% agar in glycol-water mixture; Beverloo and Weldring, 1964 — 1% agar in water; Uno and Hayakawa, 1980b — 8% bentonite in water; Baghe-Khandam and Okos, 1981 — 3.5% glass wool in water; Poulsen, 1982 — 17.5% binder, 22.5% sucrose in water; Peterson and Adams, 1983 — 10% bentonite in water).

Suspensions of 8 to 10% bentonite (a montmorillonite clay, Niekamp et al., 1984) have been the predominant model system used in the area of thermal processing. Another inhibitor commonly used is 1 to 5% agar, however, because of the low melting point (80-95 deg C) of an agar gel, it is not suited for thermal processing studies. Other gums, including sodium alginates (Glicksman, 1976) are stable at higher temperatures.

Baghe-Khandam and Okos (1981) used a novel way of preventing convection currents during heating (25 - 130 deg C), by adding glass wool ($\alpha = 2.26 \times 10^{-6}$ m^2/s) to the water (3.5% glass wool). The glass wool α is only a factor of 10 higher than that of water. Using the same set-up as Baghe-Khandam and Okos (1981), Choi and Okos (1983) measured α for water and their results agreed very well with that of published data. Gaffney et al., on the other hand, did not use water at all, but an acrylic plastic ($\alpha = 1.30 \times 10^{-7}$ m^2/s), having thermal properties very close to those of food products.

Published Values of Thermal Diffusivity

Published lists of thermal diffusivity values for foods are few (Gaffney et al., 1980; Poulsen, 1982; Singh, 1982), and most well known food engineering textbooks do not include these lists. When α values are published, the temperatures at which α was measured, the moisture content of the food item, and the uncertainty of the results are generally not reported (Martens, 1980). The temperature range for which α is measured can be very important. Martens (1980) showed that lethalities calculated for pouches, using α values obtained at the high and low temperature range of the process give a difference in the final bacterial concentration as high as one billion to 1. Martens (1980) also showed that the moisture content of a food product dictates the product α value much more than any of its other constituents (i.e., fat, protein, and carbohydrate).

An important point that Martens (1980) puts forth, which will not be discussed here but deserves investigation for cans, is that when using a constant α value when calculating lethalities of a process in a pouch, large errors in the final survivors population can occur. Factors of a thousand to 1 or more in difference were observed for lethalities calculated from constant α values obtained from the low and high temperature range of the process as compared to a temperature dependent thermal diffusivity equation. Such variations in process lethality could potentially result in over-, or worse, under-processed foods.

Theoretical Development

Taking into consideration the results of Chapter 1, equations (3) and (6) are used as the model for estimating . If the surface heat transfer coefficients are known to be different from infinity, then the appropriate equations are used. When heat conduction along the thermocouple is assumed to be in a quasi-steady state condition (boundary conditions change slowly enough so that the heat conduction along the thermocouple can be modeled as a steady state problem), the temperature of a radially mounted probe can be described with the equation

$$\frac{d^2T(r,t)}{d^2r} - \frac{hP}{kA}\left[T(r,t) - T_c(r,t)\right] = 0 \qquad (11)$$

with

r = distance from the outside surface; $r = R$ at tip of probe

h = surface heat transfer coefficient between the probe and the food item

P = perimeter of probe; $P = 2\pi R$

A = cross sectional surface area of probe

k = thermal conductivity of probe

$T_c(r,t)$ = temperature of surrounding food item at position r and time t

$T(r,t)$ = temperature of probe at position r and time t.

The analytical solution (Appendix A) to equation (11) with $r = R$ (center of can) is

$$\theta^*(t) = \theta(t)\left[1 + \frac{2e^{-m'R}}{(m'R)^2}\left[\tanh(m'R) - 1\right] + \frac{2}{m'R}\left[\frac{1}{m'R} - \tanh(m'R)\right]\right] \tag{12}$$

with

m' = probe factor $\sqrt{hP/kA}$

R = radius of can

$\theta(t)$ = temperature of food item at center and time t calculated from the analytical solution to Fourier's heat conduction equation (equations 3 and 6)

$\theta^*(t)$ = adjusted actual temperature at time t and at center of can

When the probe factor is large ($m'R > 100$), equation (12) reduces to

$$\theta^*(t) = \theta(t)\left[1 + \frac{2}{m'R}\left(\frac{1}{m'R} - 1\right)\right] \tag{13}$$

With the use of equation (12) or (13) and (3) and (6) the probe factor can be estimated from a thermal process for a product with known α. Once the probe factor is known, can be estimated from thermal process data of food items.

Experimental Procedure

A 2% water-KELSET, a sodium-calcium alginate, solution was sufficient to prevent any convection heating during a thermal process (KELSET is distributed by Kelco, a division of Merck and Company Incorporated). The KELSET solutions were prepared by measuring a volume of deionized water to which a 3% (by volume) 2 normal solution of HCl was added. The hydrochloric acid prevented the KELSET from thickening during mixing. The low pH water was stirred with a rotary mixer at a high speed during which the KELSET was added very slowly, to prevent lumping. After the KELSET had been added, an equal amount of 2 normal NaOH was added to neutralize the solution. Upon neutralization, the solution thickened to a pourable jell. With the use of the acid and the base, incorporation of air was minimized.

KELSET was chosen for use because of its very high viscosity at low solids content and because it retains much of its viscosity during a thermal process. It was found that multiple processing (greater than 3) caused the KELSET to break down and lose its highly viscous character, as shown by an increase in convection heating and a resulting increase in apparent α (Table 4). Because of this, the KELSET mixture was never heated more than once (a maximum of 1 run per sample) for any of the data collection runs.

Table 4

Diffusivity value for repeated thermal processes of the same KELSET sample

Run	Diffusivity (m^2/hr)
1	.000592
2	.000594
3	.000595
4	.000622

Temperature measurements for a thermal process are predominantly taken using the "nonprojecting" Ecklund thermocouple (Ecklund, 1949). The "nonprojecting" feature of this probe causes the probe to be recessed into the can, preventing damage during can sealing. Heat conduction errors due to the presence of the Ecklund thermocouple were demonstrated by Ecklund (1955) and alluded to by Teixeira et al. (1975). Ecklund (1955) used surface mounted probes in an attempt to eliminate the temperature measurement error due to the probe.

To investigate the effect that the bias temperature values have on the estimation of α, temperature measurements were done with both an Ecklund thermocouple and a mineral insulated probe. The mineral insulated probe used was a type T thermocouple, manufactured by LOVE Controls Corporation (part no. 1818-57). The sheath of the probe was made of type 304 stainless steel and allowed for an exposed junction. The mineral insulated thermocouple was mounted on the can with the use of a nylon fitting ($\alpha = 1.136 \times 10^{-7}$ m^2/s), made specially for this research project. After mounting and before can filling, the probe was accurately positioned in the center of the can. The cans were all filled as full as possible to eliminate any head space effects.

Three can sizes (Table 5) were used for this portion of the research: 303x406, 307x409 (No. 2), and 401x411 (No. 2 1/2). The 303x406 was used because the Ecklund thermocouples available were for this size can. The 307x409 and 401x411 cans were used because of their size, as suggested in Chapter I, and to investigate whether or not the difference in L/R ratios influenced the results significantly.

Table 5

Can sizes used for data collection

Can Number	Radius (R) (m)	Half Height (L) (m)	L/R
303x406	.0383	.05250	1.370
307x409	.0417	.05575	1.340
401x411	.0516	.05650	1.141

All experiments were done in one of two still retorts. When possible a mini-retort was used (radius of .13m, length of .22m), to minimize the come-up time (less than 10 seconds). Due to the small size, only the 303x406 can fitted into the mini-retort. For runs using the 307x409 and 401x411 cans a pilot-plant size retort was used (radius of .45m, length of .67m). The come-up time on the pilot-plant retort was always less than 90.0 seconds and not considered significant.

Data was collected for each run using a Hewlett Packard Model 3045DL data acquisition system. Data for each (if more than one) of the cans, in addition to the retort temperature, was collected at 45 sec intervals for the duration of the test. A test run was considered complete when the temperature ratio difference between the retort and the food item fell below 0.10. The data was stored on a magnetic tape and was later uploaded to a main-frame computer for analysis. The programs discussed in Chapter I were used for the analysis. Only the data that fell within the θ range of 0.15 to 0.85 was used for the estimation of α.

Surface heat transfer coefficients (h) for each of the retorts were measured using a finite cylinder made of copper. The dimensionalized Biot Numbers (h(V/A)/k) associated with the copper cylinder (0.17) allowed for the estimation of h using the same programs as used for the estimation of α. Before being placed into the retort, the copper cylinder was kept in a water bath for over two hours to establish a uniform initial temperature. Immediately, upon transfer from the water, the retort was sealed and started, during which time data was collected every 5 seconds.

To establish an estimate of precision in estimating α from thermal process data, 25 runs for each can were done using the KELSET model system. These same runs, 75 total, were used to estimate the probe factor associated with the thermocouples used. KELSET was also used to make two runs haveing an 8 min come-up time and a known can head space. A number of food products were also tested. Each of the food items were purchased from a local supermarket or donated by a manufacturer. Peas and lima beans were pureed before analysis by blending the entire contents of the can at a high speed until smooth. The mashed potatoes were reconstituted from potato flakes to the desired moisture content. The apricot sample was a strained baby food puree. The moisture of each sample was measured using a vacuum oven set at 100 deg C and dried to a constant weight.

Results and Discussion

Surface Heat Transfer Coefficients of the Thermal Process

Attempts were made to measure the surface resistance (h) of a can heated in a steam environment. Thermal resistance due to heat penetration through the can and due to the contact resistance of the product and can could not be estimated. Using a solid copper cylinder with known dimensions and thermal properties, time-temperature heating curves were measured. The duration of each test was 60 to 100 seconds. Since the time required to place the copper cylinder in the retort, seal it, and to establish pressure (15psig) took 15 to 20 seconds, simulation of a step-change in surface temperature was not possible. The result, then, was that any estimate of the surface resistance would be low. An average surface resistance of about 3700 W/m^2C was measured for a number of runs. This corresponds to a dimensionalized Biot number (h(V/A)/k) of 85.0 for the 307x409 can. Considering the fact that this value is low and that Ramaswamy et al. (1983) reported h values of 11,000 W/m^2C for condensing steam, the surface resistance was considered infinite (Bi greater than 200) for all the experimental runs reported in this study.

Errors in Estimating Diffusivity

Twenty five runs for each of the three cans listed in Table 5 were done using 2% KELSET solutions. All 25 of the tests using the 303x406 can and Ecklund thermocouple were run in a mini-retort. The rest of the tests, including those for the food products, were done using the pilot plant retort. The larger retort allowed for multiple tests, but had a longer come-up time. When KELSET was used, it was made fresh for each run, except those mentioned in Table 4. Many of the food products were canned, processed, allowed to sit overnight (to equilibrate to room temperature) then reprocessed.

Applying the results from Chapter I, only the data between the temperature ratio (θ) range of 0.15 to 0.85 was used when estimating α from the thermal process data. The trends of a typical residual (actual temperature - the calculated temperature) plot obtained from any of the tests is presented in Figure 21. The amount of scatter varied with each test, but in all the cases definite trends in the residuals were noticeable. Three general types (A,B,C) of trends were obtained from the tests. All three types demonstrated a large underestimation of temperature at low time, which decreased to an overestimation after longer time periods. Differences in the plots were present only at the end of the heating. Type A plots had a large underestimation in temperature at the end of the heating period. For type B plots only a slight underestimation occurred after the overestimation, and for type C plots the overestimation remained relatively constant until the end of heating.

To draw statistical conclusions from a regression analysis, a number of assumptions are made concerning the data. The more important assumptions are: 1) the residual error has a zero mean, 2) the errors are additive, and 3) the errors are independent and identically distributed. For the estimation of α from thermal process data, assumptions 1 and 2 can be readibly assumed from the model. However, from Figure 21 the residuals show a very strong correlation and, thus, are not independent. A number of factors could cause this dependence. The first is that the model may not adequately describe the data and the second is that the data is in fact correlated.

Schisler (1979) showed that transient heat conduction data collected rapidly, over a short period of time, showed autocorrelation in the errors. Since the sampling rate was low, 1 data point every 45 seconds, any autocorrelation due to sampling can be neglected. From inspection of the collected data, it became apparent that the lag time period was much shorter than expected, indicating that the model does not properly describe the data. This lack of lag time resulted in an underestimation of temperatures of 1.0 to 3.0 deg C at low time periods. The underestimation could be the result of: 1) convection heating, 2) temperature dependent thermal properties, and 3) heat conduction along the thermocouple wire. In considering the results for the copper cylinder, a finite surface heat transfer coefficient is ruled out because it would cause the lag time to increase and not decrease.

To determine if convection heating was present during the thermal process, a very thick and non-flowable food product (pumpkin puree) was processed. Residual trends identical to Figure 21 were obtained for ten different runs. These results, in addition to showing that the trend in residuals is not due to convection heating, demonstrated that the 2% KELSET solutions are very adequate in preventing convection heating of water.

If the temperature dependent thermal properties were the cause of the large underestimations in temperature at low time, the thermal property values would have to start high and decrease with heating. Gaffney et al. (1981) and Choi and Okos (1983) present data and models for the thermal diffusivity of water at different temperatures. Both diffusivity models indicate that the α of water increases with temperature and does not decrease. Thus, thermal properties of water will start low and increase — just the opposite of what is needed to account for the short lag time.

Beverloo and Weldring (1969) measured the error associated with heat conduction along a radially mounted thermocouple and showed that the errors rapidly increased

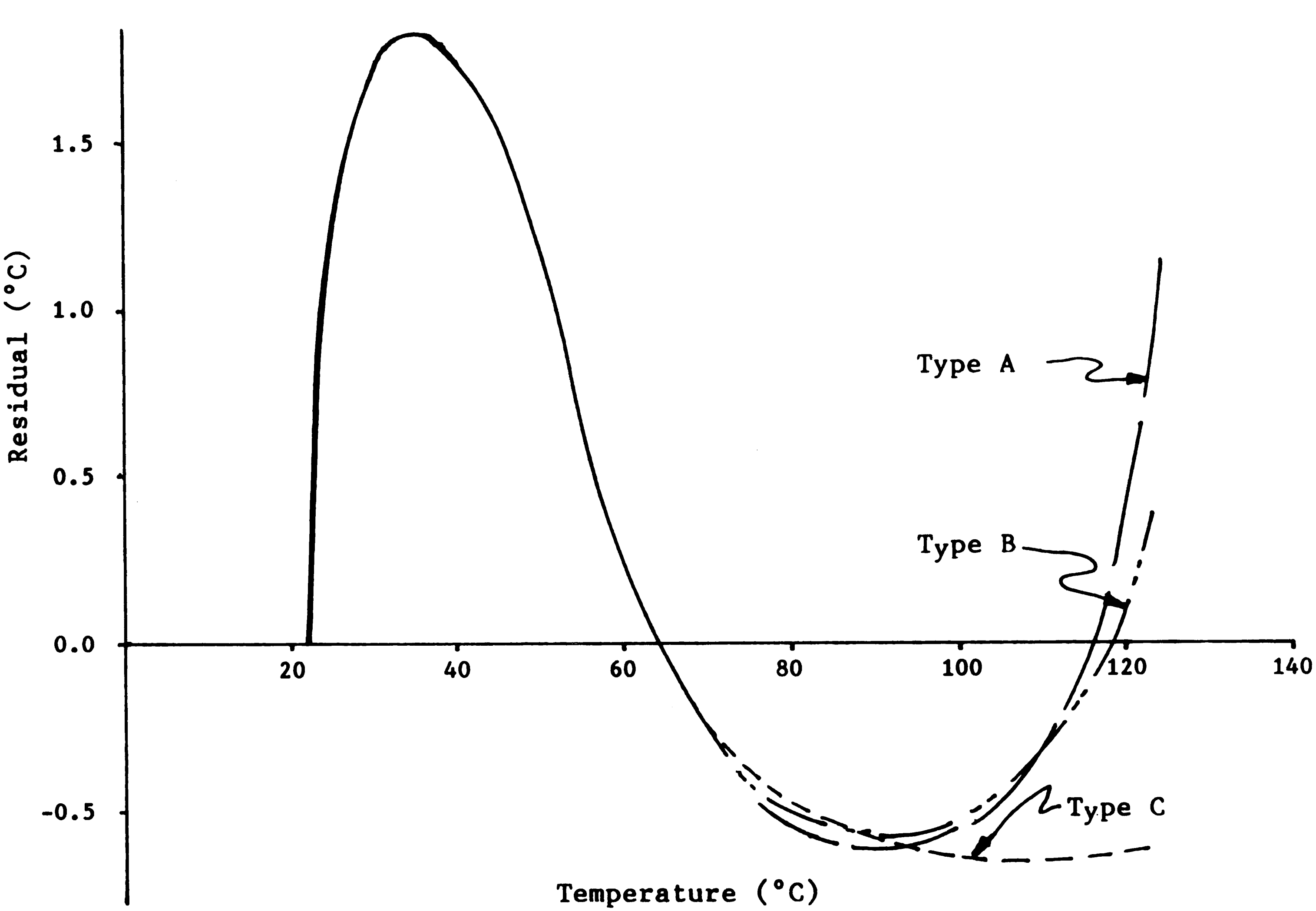

Figure 21. Residual error trend of the estimation of diffusivity from thermal process data.

from time zero to a maximum shortly afterward and then asymptotically returned to zero. The shape of the error in the temperature measurement curve that Beverloo and Weldring (1969) measured for 16 different thermocouples is exactly like the type C curve in Figure 21, the only difference being that, by regressing the data to obtain α, the error in temperature measurement has been brought below zero after long time periods. If the curves in Figure 21 were due to errors in temperature measurements because of heat conduction along the thermocouple probe, the estimated values of α would be higher than they actually are.

Correcting for Errors in Temperature Measurement

Table 6 lists the average (of 25 runs, Appendix B) α values for each of the can sizes in Table 5. Taking into consideration only the temperatures of a thermal process between the θ range of 0.15 to 0.85, the average α value for water is .5915 x 10^{-3} m^2/hr. From Table 6, it can be seen that α was consistently estimated higher than that for water, when it was estimated using only the analytical solution to Fourier's heat conduction equation (α_1, in Table 6). By incorporating a correction factor (m') for the heat conduction along the thermocouple probe (equations 3,6, and 12), a noticeable reduction in the estimated α values can be seen (α_2, Table 6). Considering a 95% confidence interval ($t_{.95}(25) = 2.06$) for α_2, water α falls well within the confidence region for each can size (303x406, $.586 < \alpha_2 <$

.611; 307x409, .586 < α_2 < .607; 401x411, .584 < α_2 < .600). In comparison, the 95% confidence region for α_1 included the α value for water (303x406, .592 < α_1 < .613; 307x409, .597 < α_1 < .624; 401x411, .589 < α_1 < .607) with only the 401x411 can.

Table 6

Average estimated diffusivity values for 2% KELSET solutions. (α_1, estimated using equations 3 and 6; α_2, estimated using equations 3, 6, and 12; α_3, estimated using equation 10)

Can size	α_1 $\times 10^3$ (m^2/hr)	MSE (C)	α_2 $\times 10^3$ (m^2/hr)	m´ (m^{-1})	MSE (C)	α_3 $\times 10^3$ (m^2/hr)
303x406						
x	.6023	.0632	.5987	5001	.0295	.6016
S_x	.00502	.0274	.00595	1153	.0313	.0188
307x409						
x	.6107	.3267	.5973	1884	.00294	.6009
S_x	.00677	.246	.00471	488	.00328	.0178
401x411						
x	.5989	.0987	.5918	3864	.0108	.6106
S_x	.00448	.096	.00398	1680	.0277	.0233

From Table 6, it can be seen that a reduction in the estimated value of α was accompanied by a reduction in the mean square error (MSE) of the estimate. MSE is the sum of the squared difference between the actual and calculated temperatures divided by the number of data points minus the number of estimated parameters. Therefore, MSE gives an indication of how well the model fits the data: the smaller the MSE, the better the fit.

Figure 22 depicts the three general types of residual trends that were obtained when estimating both α_2 and m´. Here again, as for Figure 21, scatter was dependent on the test run, only the size of the scatter either increased or remained the same. The type D curve of Figure 22 resulted from an unchanged residual plot of Figure 21 (type A) and an unchanged MSE value. For the cases when the MSE was unchanged, the probe factor (m´) was large and could be considered negligable. The type D curve of Figure 22 appeared a number of times for the 303x406 can (which used the Ecklund thermocouple) and a few times for the larger 401x411 can. All of the type C curves (Figure 21) were reduced to type F curves (Figure 22) with the incorporation of m´. The intermediate B curves of Figure 21 resulted in mostly type E to F curves when m´ and α were estimated. The significance of m´in smoothing out the residual plot was directly related to the size of the upward curved portion of Figure 21 at the end of the heating period.

There is a large error between the predicted and actual temperature at the beginning of the heating period (Figure 22). These error values are a result of a quasi-steady state assumption used in deriving equation (12) (Appendix A). It is assumed that the thermocouple temperature changes within itself at such a rate, as compared to the food

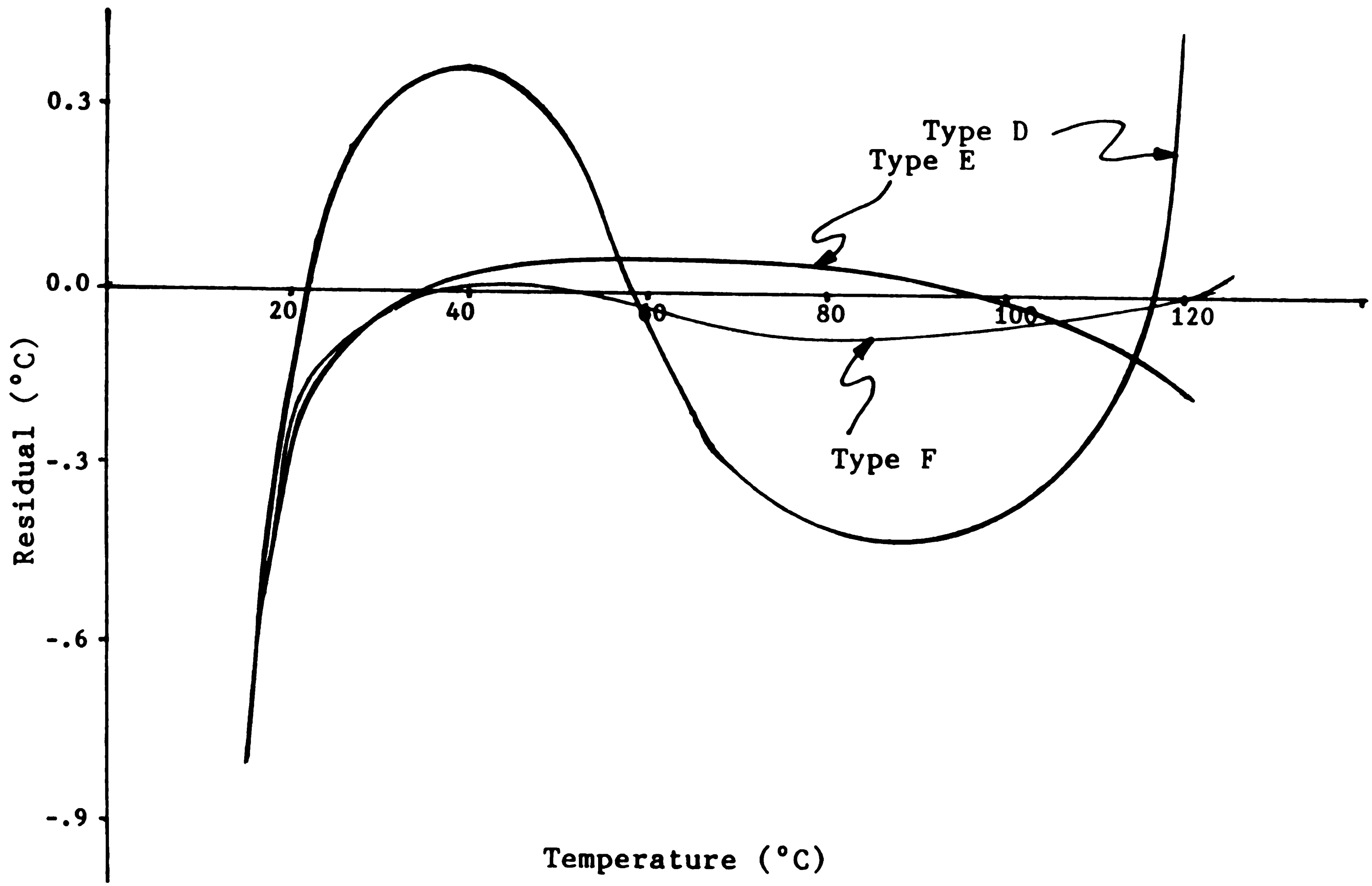

Figure 22. Residual error trend of the estimation of diffusivity corrected for heat conduction along the thermocouple, from thermal process data.

product, that it can be assumed to always be in a quasi-steady state with its surroundings. Since this assumption is not true at low times, equation (12) will tend to cause the model to predict temperatures larger than the actual values. This overestimation of temperature at the beginning of heating does not influence the estimate of α because the assumption remains valid for the thermal process data that falls between the θ range of 0.15 to 0.85. At θ = 0.85 and t = .25hr the Fo value for the thermocouple (α = .0792 m^2/hr, value for stainless steel) is greater than 5.0 for all of the cans considered in Table 5. This means that the thermocouple has essentially reached equilibrium with its surroundings.

The temperature difference compensated for using equation (12) is presented in Figure 23. The temperature difference ratio ($\Delta\theta$) was calculated as the difference between the corrected temperature ratio (equation 3,6, and 12) and the temperature ratio calculated using just the analytical equations (equation 3 and 6). The slope of the lines are dependent on both the m' value and the dimensions of the can. However, for the three can sizes in Table 5, differences between the plots were small. The curves in Figure 23 are straight lines, meaning that equation (12) will tend to compensate on a linear basis; thus, the best compensation is found for the type C in Figure 21.

The Beverloo and Weldring (1969) curve for the error in temperature measurement of a radially mounted probe, as

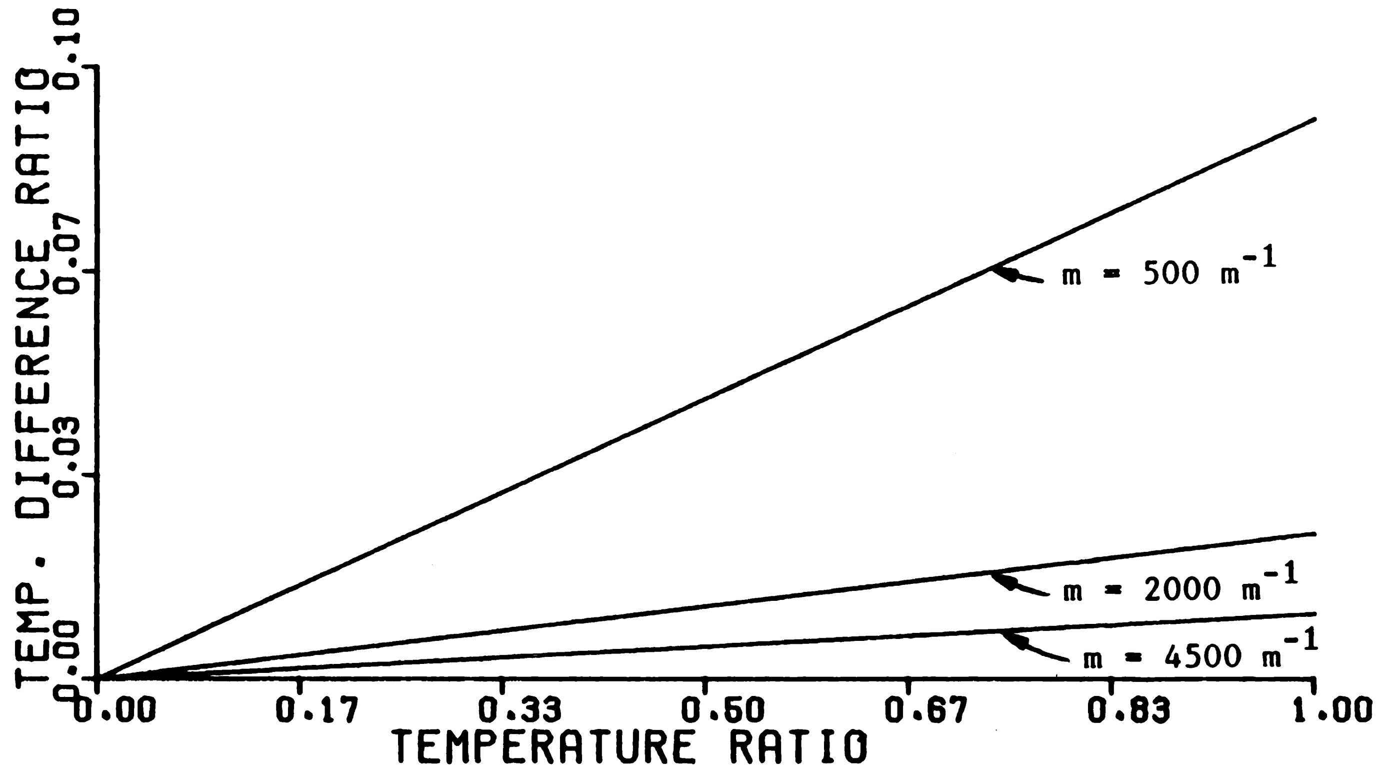

Figure 23. Difference in temperature ratio resulting from correction of heat conduction along the thermocouple probe, for three different probe factor values (m´).

indicated before, was not a straight line, but a parabola. Thus, a correction model for heat conduction down a thermocouple should be a parabola and not a straight line as in Figure 23. Before a different correction model is proposed or even equation (12) is considered, the question of its importance needs to be asked. Table 7 (Appendix B)

Table 7

Average difference between diffusivity values of 2% KELSET solutions (α_1, estimated using equations 3 and 6; α_2, estimated using equations 3, 6, and 12; α_3, estimated using equation 10)

Can size	$\alpha_2-\alpha_1$ x10^3 (m^2/hr)	%difference $(\alpha_2-\alpha_1)/\alpha_2$	$\alpha_2-\alpha_3$ x10^3 (m^2/hr)	%difference $(\alpha_2-\alpha_3)/\alpha_2$
303x406				
x	-.0037	-.612	-.0029	-.463
S_x	.0026	.436	.0142	2.34
307x409				
x	-.0134	-2.25	-.00367	-.603
S_x	.00431	.715	.0143	2.40
401x411				
x	-.0062	-1.05	-.0188	-3.17
S_x	.00363	.614	.0209	3.52

presents the percentage difference in α when estimated with and without equation (12). The correction (2.25%) is largest for the 307x409 can. Since 5% variation in estimated thermal properties of food items is not unreasonable, the importance of correcting for heat conduction along the thermocouple probe seems small. When different can sizes are used, the correction will become more important as the L/R ratio increases. Therefore, whenever α is being estimated from a thermal process using a radially mounted probe, the magnitude of the error associated with the radially mounted probe should be assessed. The magnitude of m' is especially important for small cans and for ones that have a large L/R ratio.

Figure 24 presents the sensitivity ratios plotted aganist the θ for the model consisting of equations (3), (6), and (12). Sensitivity plots were made for the same can sizes used for the sensitivity analysis in Chapter I and for m' values ranging from 1000 to 5000 m^{-1} (a total of 9 plots). Each plot was essentially the same as the other. As can be seen from Figure 24, the coefficients are not correlated. Correlation exists if for at all times the two curves differ by a constant. The magnitude of the sensitivity coefficients values are different by an order of 1 to 17 for m equal to 1000 (m^{-1}) and an order of 1 to 85 for m' equal to 5000 (m^{-1}). Therefore, when estimating both α and m' simultaneously, the estimate of m' will probably have a larger standard deviation than that of α. Considering the small importance (only a 2% difference in α) of m', the importance of its estimation is low. Therefore, even though residual plots like those in Figure 21 may exist for the estimation of α, any corrections made in the model

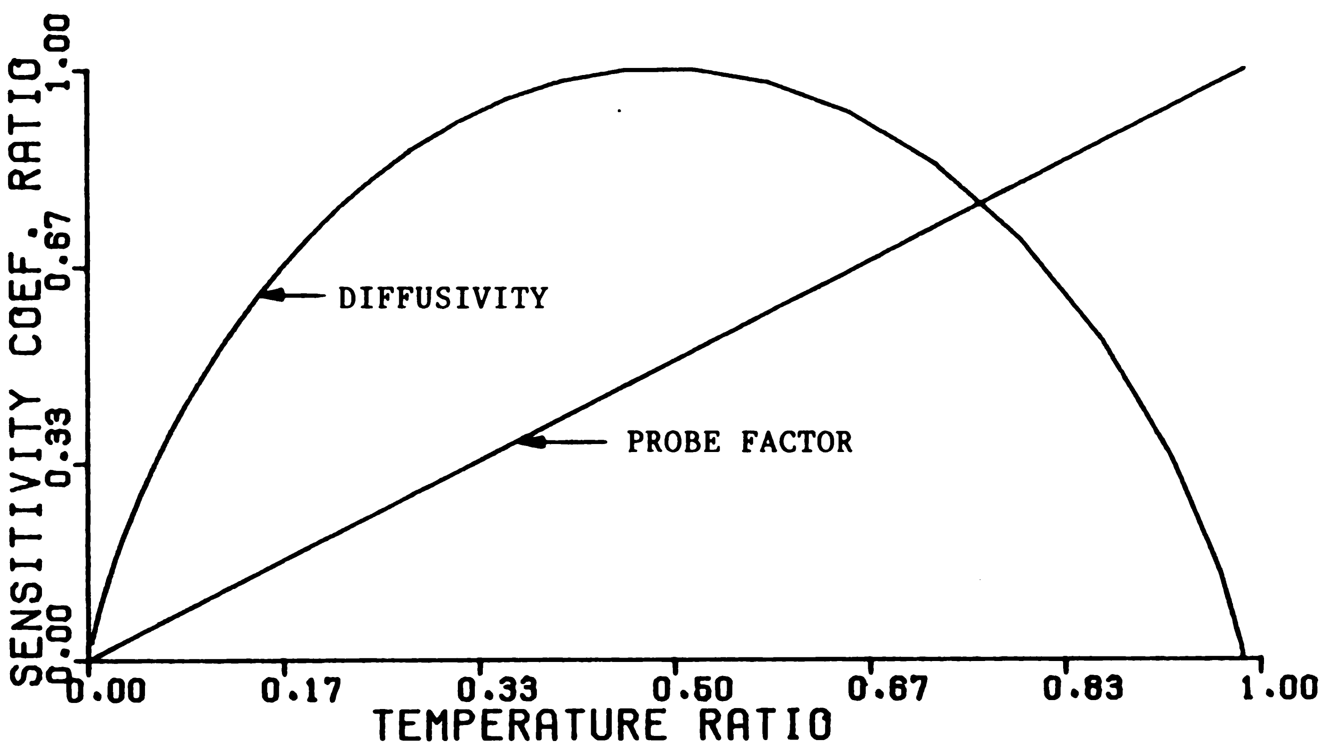

Figure 24. Sensitivity coefficient ratio as a function of temperature ratio for diffusivity and for a probe factor, estimated simultaneously from thermal process data.

used in estimating α (i.e., incorporation of a probe factor) will in many cases not change the estimate. However, before neglecting a correction factor for heat conduction along the thermocouple, a researcher should determine the magnitude of the error in temperature measurement due to the probe and, if significant, compensate for it in the model.

Errors from Devient Thermal Processes

A few thermal process runs were made with a long come-up time (8 mins, a typical come-up time of a production scale retort) and for cans containing a 1.27 cm head space (measured from the lip of the can before sealing). Upon analysis the 307x409 can demonstrated no significant change in α (α = .5927 x10^{-3} m^2/hr) for a 1.27 cm head space when estimated using the analytical solution (Appendix D). The reason for this is that the large L/R ratio caused most of the heat to penetrate radially. Diffusivity, when estimated from f_h, showed a significant decrease in the estimate as compared to the other estimates of α. The magnitude of decrease in α increased for the 401x411 can when compared to the 307x409 can. This is because the L/R ratio for the 401x411 can is smaller. Still, even with the larger decrease in α for the 401x411 can, the difference in the α from those in Table 6 is only 1.6%. However, when looking at the α estimated from f_h the difference is 3.9%.

The 8 minute come-up time caused a significant reduction in the estimated α (.5621 x10^{-3} m^2/hr). The residuals of the regression were much different from those of the other estimations, indicating that the model was not fitting the data well. Diffusivity estimated from f_h, on the other hand, did not indicate any problems with the data or the model. The conclusion is that commercial retorts, which typically demonstrate come-up times of this nature, should not be used when collecting thermal process data used in estimating α.

Estimating Diffusivity from Olson and Jackson Equation

Tables 6 and 7 present the results of estimating α (α_3) from f_h using equation (10), the Olson and Jackson (1942) equation. These tables indicate, that when using f_h, the estimate is high, as expected from the results in Table 3. More importantly, the estimates have a standard deviation 3 to 5 times that found for α estimated from the analytical solution to Fourier's heat conduction equation. With C_v values of 3.0 to 3.8% as compared to the C_v of α (0.7 to 1.1%) estimated using the analytical solution to heat conduction, the estimates of α from the Olson and Jackson equation (equation 10) are inadequate. The inadequacy of equation (10) is even more pronounced when the product being analyzed deviates from a solely conduction heating product.

Table 8 presents the α values estimated from four different thermal process runs of mayonnaise, which exhibited no obvious change in consistency. The estimates for α using the analytical solution are different from the estimates of α using the Olson and Jackson (1942) equation by 20% (Table 8). Figure 25 shows that the predicted

Table 8

Estimated values of α for mayonnaise (α_1, estimated using equations 3 and 6; α_2, estimated using equations 3, 6, and 12, m'=1900 m^{-1}; α_3, estimated using equation 10)

Run	α_1 $x10^3$ (m^2/hr)	MSE (C)	α_2 $x10^3$ (m^2/hr)	MSE (C)	α_3 $x10^3$ (m^2/hr)	%difference $(\alpha_2-\alpha_3)/\alpha_2$
1	.4104	14.99	.4007	10.37	.3136	21.74
2	.4168	16.53	.4070	11.56	.3178	21.92
3	.4022	16.59	.3933	11.92	.3158	19.71
4	.4112	14.57	.4022	10.28	.3275	18.57
x	.4101	15.67	.4008	11.03	.3187	20.49
S_x	.00602	1.04	.00568	.830	.00613	1.62

temperatures using the analytical model (equations 3 and 6) do not follow the actual temperatures very well. This can also be seen from Table 8 by the large MSE values. Because of this deviation, it is safe to assume that the mayonnaise did not heat by pure conduction. Figure 26 shows that, even though mayonnaise heats with convection, the slope of the heating curve (f_h) does not indicate this heat transfer mode. When looking at Figure 25 it can be seen that the estimated α from Figure 26 (f_h) is in gross error because it badly underestimates the temperature of the mayonnaise when it is used in the analytical solution to the Fourier heat

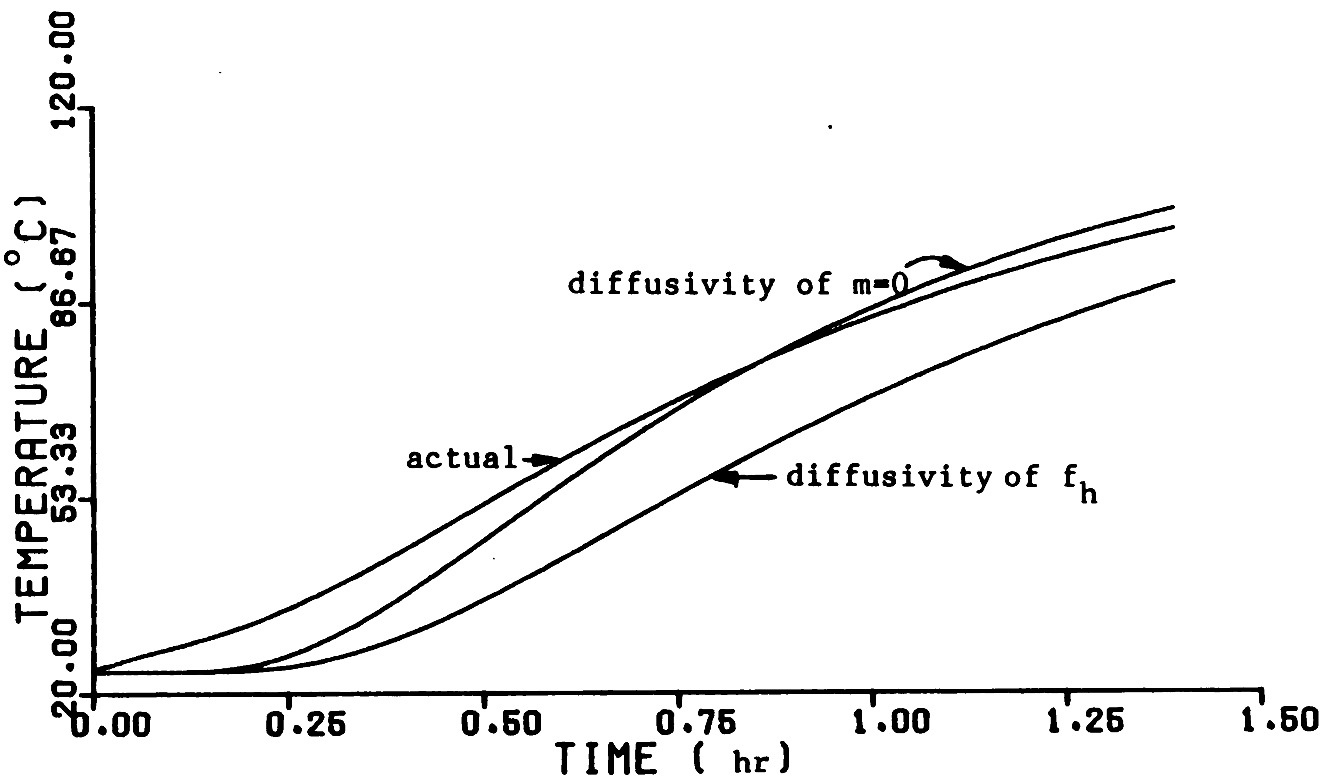

Figure 25. Actual and calculated temperature values for mayonnaise using diffusivity values estimated from the analytical solution and from f_h.

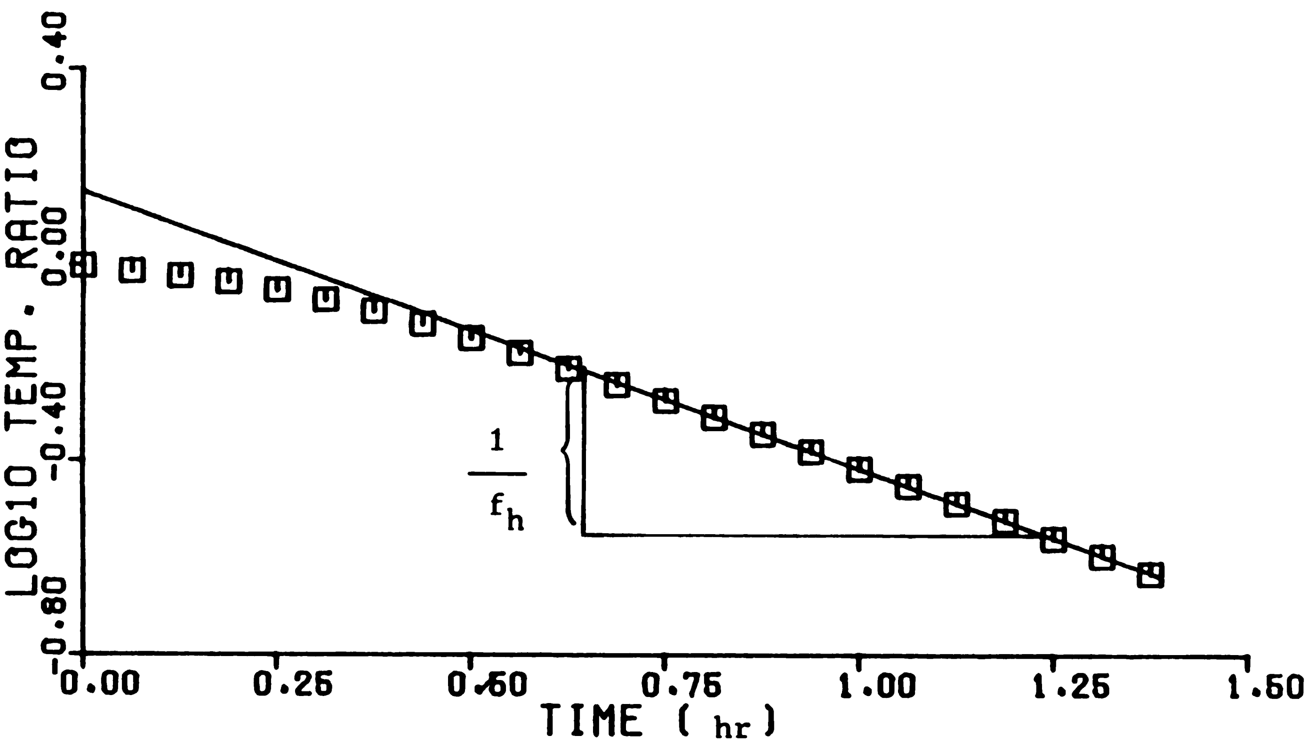

Figure 26. Log_{10} of temperature ratio as a function of time for calculation of f_h for mayonnaise.

conduction equation. Since α is used in conjunction with the analytical solution to heat conduction, it would be wise not to use α values calculated from f_h, unless the user knows for sure that convection heating is not present and is not that concerned with calculated values having a large standard deviation.

Diffusivity of Actual Food Products

Diffusivity was estimated for a number of food products using equations (3), (6), and (12), and their average values are presented in Table 9 (Appendix C). The probe factor was assumed to be equal to 1900 (m^{-1}) which was the average value estimated from the 2% KELSET solutions in the 307x409 can, the same can used for all the food product testing. In addition to the α values obtained during this study, some α values obtained from previously published literature are reported in Table 9. Comparison between α calculated in this study and previously published values is difficult due to moisture content differences and the differences in temperature ranges used in estimating α. However, when one realizes that a decrease in moisture content will decrease the estimated α and that an increase in the temperature of the heating media will increase the estimated α, some generalizations can be made.

Poulsen (1982), using the regular regime method, obtained α values for apple sauce that are lower than the α value estimated from this study. Since the apple sauce used

Table 9

Estimated diffusivity values for tested food items (average values; can size 307 x 409, $m' = 1900m^{-1}$) and from previously published papers.

Product	Moisture %	Temp. Range ^{o}C	α ($x10^{3}$) $m^{2}/hr.$	Reference
Apple Sauce	82.0	20-121	.5612	this study
	75.7	21-50	.5418	Poulsen (1982)
	80.0	65	.5040	Riedel (1969)
	--	26-126	.6000	Lenz and Lund (1977)
Baked Beans	70.0	20-121	.5490	this study
	--	26-126	.6039	Lenz and Lund (1977)
Lima Bean Puree	80.1	20-121	.5707	this study
	--	26-126	.6465	Lenz and Lund (1977)
Mashed Potatoes				
(reconstituted)	73.5	20-121	.5755	this study
(reconstituted)	81.5	20-121	.5793	this study
(reconstituted)	88.2	20-121	.5781	this study
(cooked)	78.0	65	.5613	Riedel (1969)
Mayonnaise	16.9	20-121	.4008	this study
	16.9	20-121	.3187	this study-f_h
	18.0	22-50	.3834	Poulsen (1982)
Pea Puree	84.4	20-121	.5783	this study
	--	26-129	.6542	Lenz and Lund (1977)
	--	25-121	.6116	Teixeira et al (1975a)
Potato Salad	74.7	20-121	.5477	this study
	--	1.7-80	.5187	Dickerson and Read (1968)
Pumpkin	--	20-121	.5733	this study
Tomato Juice (average)	73.0	30-121	.504	Choi and Okos (1983)
Tomato Paste	73.1	20-121	.5455	this study

by this study had a higher moisture content and was evaluated at a higher temperature, the difference in values does not seem too great. Conversely, Lenz and Lund (1977) reported α values for apple sauce that are higher than those found in this current work. The high estimation of α found for all of their reported values. In fact, all of the α values reported by Lenz and Lund (1977) are higher than that of water, where the reverse trend should be the case (Choi and Okos, 1983). Thus, the validity of the Lenz and Lund (1977) data is questionable.

In an attempt to study the effect of moisture on the α of mashed potatoes, 3 different samples of mashed potatoes were made by reconstituting potato flakes with water. The variation in moisture ranged from 73.5 to 88.2%. Values of α estimated from the three samples do not demonstrate any trend related specifically to moisture content.
Diffusivities of tomato juice concentrates were estimated by Choi and Okos (1983) for a large number of moisture contents. The data showed a decrease in the diffusivity of the tomato juice with increasing solids. The rate of change was slow for solid contents ranging from 4.8 to 20% and then was much more rapid as the solids content increased to 80%. Due to a difference in moisture of only 15% for the mashed potato samples and the overall high moisture content, it is not surprising that the change in moisture contents had little influence on estimated α values.

It seems apparent from Table 9 that, due to the large variability in reported α values for the same product, α should be measured for each product studied. Since thermal process data is easy to collect, the procedure outlined in this study would be a reliable, fast, and easy method to use in estimating α.

Summary and Conclusions of Experimental Analysis

Temperature measurement errors due to the presence of a thermocouple will cause the residuals of the estimated α values to be correlated (Figure 21). By compensating for the heat conduction down the thermocouple, a reduction in the residuals will occur along with a reduction in autocorrelation (Figure 22). The difference in α estimated with and without compensating for temperature measurement errors depends on the size and shape of the can (Table 6). Larger cans with small L/R ratios will yield more accurate temperature measurements due to the reduced influence of heat flowing radially into a can and down the thermocouple. Estimations of α with Ecklund thermocouples having metal fittings do not appreciably differ from α estimated using data collected with a small diameter probe having nylon fittings. No matter what type of thermocouple is used in estimation of α, a researcher should first establish that it does not significantly affect the estimate before its presence is neglected.

When estimating α from thermal process data collected in a steam environment, the boundary conditions are usually easily established. A small retort with adequate steam lines, to reduce come-up time, should be used. Head space effects can be easily eliminated by filling the can as full as possible. It is best to set up individual experiments when estimating α from thermal process data and not from routine thermal process analyses.

Thermal diffusivity estimated from the logroithmic portion of the heating curve (f_h) will result in estimates with the following characteristics: 1) larger standard deviations than those found using more analytical methods (Table 6), 2) estimated values that could be the result of unknowingly having unsatisfied boundary conditions, such as long come-up times, and 3) potentially inaccurate estimates resulting from the presence of convection heating (Table 8). For cases where a long come-up time, a head space, or convection heating is present the logorithmic portion of the heating curve will remain linear, indicating no problems in the estimate. Thus, misleading the researcher into using values for α that are potentially inaccurate.

Thermal diffusivity of actual food products will fluctuate with moisture content and temperature. Due to this fluctuation, one should use caution if using published α values (Table 9). In turn, α should be measured for each product investigated.

Considering the experimental data collected in this chapter, the following estimation guidelines should be included in any thermal process procedure used in estimating α:

1) Use a 401x411 or larger can to reduce errors associated with heat conduction down the

thermocouple probe (when consistent with the thermocouples used in this analysis).

2) Maintain the head space in the can to a minimum, especially for cans with a small L/R ratio.

3) Keep the come-up time of the retort to a minimum. Come-up times less than 2 minutes are adequate when considering canned food products of the size used in this study.

4) Investigate the residuals of the estimated α for trends - indicating nonconformity to the boundary conditions imposed on the model. This is particularly helpful in determining if convection heating is present.

5) Estimating α from the slope of the heating curve (f_h) may result in poor estimates and is not a recommended practice.

RECOMMENDATIONS

Recommended Estimation Procedure

Estimation of thermal diffusivity is more accurately accomplished using the analytical solution to the Fourier heat conduction equation and to a lesser extent by the regular regime method. Any incongruities in the data are best observed by using the analytical solution and may be masked with the regular regime method.

Summarizing from the conclusions of Chapters I and II the following guidelines are recommended when attempting to estimate thermal diffusivity from thermal process data using the Fourier heat conduction equation as a model and employing the nonlinear least squares method of parameter estimation.

1) Use a can size that will minimize the importance of heat conduction along the thermocouple probe and probe misplacement. A can size of 401x411 or larger was considered adequate for this study.
2) Use a can with a L/R ratio close to 0.8 or less. This will decrease the importance of errors in can dimensions and time measurement, but more importantly will decrease the quantity of heat conducted along a radially mounted thermocouple probe.
3) Use a material with known thermal properties (Bi greater than 40) to determine the magnitude of the

surface heat transfer coefficient. If Bi is greater than 200 the surface heat transfer coefficient can be considered infinite.

4) Limit the range of data used in calculating thermal diffusivity to the temperature ratio range of 0.15 to 0.85.

5) Establish the thermal process procedures such that the temperature difference between the initial product temperature and the heating medium temperature is not lower than 40.0 deg C.

6) Maintain the head space in the can at a minimum, especially for cans with small L/R ratios.

7) Maintain the come-up time of the retort to a minimum. Come-up times less than 2 minutes are adequate when considering canned food products of the size used in this study.

8) Investigate the residuals of the estimated thermal diffusivity for trends that may indicate nonconformity to the boundary conditions imposed on the model. This is particularly helpful when convection heating may be present.

9) Thermal diffusivity should not be estimated from the slope of the heating curve (f_h) due to potentially poor estimates.

In conjunction with the above, the following standard experimental procedures are recommended when obtaining data to be used in estimating thermal diffusivity:

1) Measure, as accurately as possible, the position of the thermocouple probe after its placement and the inside dimensions of the can.
2) Use a data acquisition unit to collect data. This will minimize errors in time measurement.
3) Calibrate the thermocouple probes to minimize errors in temperature measurement.
4) Establish good operational procedures for estimating α for food products by testing the operation with a product having known thermal properties such as water with a convection heating inhibitor.

Recommended Areas of Future Study

1) Investigate the importance of accurate estimates of thermal diffusivity on the predicted loss of quality during thermal processing.
2) Investigate temperature dependency of food thermal properties.
3) Investigate how changing thermal parameter values relate to the loss of quality, rate of heating, and optimization calculations of a thermal process.
4) Investigate other mathematical models that correct for heat conduction along the thermocouple probe.
5) Determine if the temperature range used in the collection of data causes significant changes in the thermal diffusivity estimates.

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APPENDICES

APPENDIX A

Solution for model used in accounting for heat conduction along a radially mounted thermocouple in a can. Thermocouple modelled as a pin fin at a quasi-steady state.

Solution (not available in literature) to the equation

$$\frac{d^2T(r,t)}{dr^2} - \frac{hP}{kA}\left[T(r,t) - T_c(r,t)\right] = 0 \qquad \text{(A.1)}$$

which represents a pin fin in a media subject to the following assumptions:

1) the fin has a much higher thermal conductance than the surrounding media
   a) the pin has a uniform cross-sectional temperature
   b) the fin distributes its heat at such a rate that even with the changing surface temperature it is effectively always at a steady state with its environment
2) the surface temperature of the fin can be modeled using an analytical solution to Fourier's heat conduction equation
3) the temperature distribution [T(r,t)] along the fin follows a parabola (Beverloo and Weldring, 1969)

$$T(r,t) = T(0,t>0) + T(R,t)(r^2/R^2) \qquad \text{(A.2)}$$

The boundary conditions are

$$\frac{dT}{dr} = 0 \quad \text{at } r = R$$

$$T = T(0,t>0) \quad \text{at } r = 0$$

Let

$$m' = \sqrt{hP/kA}$$

$$\Delta T = T - T(0,t>0)$$

$$T_R = T(R,t)$$

Substituting A.2 in A.1, A.1 becomes

$$\frac{d^2\Delta T}{dr^2} - (m')^2\left[\Delta T - T_R(r^2/R^2)\right] \quad (A.3)$$

Splitting equation A.3 into a homogeneous part and a non-homogeneous part yields

$$\Delta T = \Delta T_h + \Delta T_i$$

$$\text{and} \quad \frac{d^2\Delta T_h}{dr^2} - (m')^2\,\Delta T_h = 0 \quad (A.4)$$

Solving for A.4 gives

$$\Delta T_h = C_1 e^{-m'r} + C_2 e^{m'r} \quad (A.5)$$

The non-homogeneous part is solved as

$$\frac{d^2\Delta T_i}{dr^2} - (m')^2\left[\Delta T_i - T_R(r^2/R^2)\right] = 0$$

Trying

$$\Delta T_i = A + Br + Cr^2$$

then

$$\frac{d^2\Delta T_i}{dr^2} = 2C$$

so

$$2C - (m')^2\,(A + Br + Cr^2) + (m')^2\,T_R(r^2/R^2) = 0$$

for this to be true

$$2C - (m')^2 A = 0 \quad ; \quad C = \tfrac{1}{2}(m')^2 A$$

$$Br = 0 \quad ; \quad B = 0$$

$$-(m')^2 Cr^2 + (m')^2 T_R(r^2/R^2) = 0 \quad ; \quad C = T_R/R^2$$

Therefore,

$$\Delta T_i = \frac{2T_R}{(m'R)^2} + \frac{T_R r^2}{R^2} \tag{A.6}$$

Combining A.5 and A.6 and satisfying the boundary conditions results in

$$\Delta T = C_1 e^{-m'r} + C_2 e^{m'r} + T_R \left[\frac{2}{(m'R)^2} + \left(\frac{r}{R}\right)^2\right] \tag{A.7}$$

$$\frac{d\Delta T}{dr} = -m'C_1 e^{-m'r} + m'C_2 e^{m'r} + \frac{2T_R r}{R^2}$$

at $r = R$; with $\frac{d\Delta T}{dr} = 0$

$$-m'C_1 e^{-m'R} + m'C_2 e^{m'R} + \frac{2T_R}{R} = 0$$

and at $r = 0$; and $\Delta T = 0$

$$C_1 + C_2 + \frac{2T_R}{(m'R)^2} = 0$$

Solving for C_1 and C_2 yields

$$C_1 = \frac{\left(\frac{T_R}{(m'R)^2} e^{-m'R} + \frac{T_R}{m'R}\right)}{\cosh(m'R)} - \frac{2T_R}{(m'R)^2}$$

$$C_2 = \frac{-\left(\frac{T_R}{(m'R)^2} e^{-m'R} + \frac{T_R}{m'R}\right)}{\cosh(m'R)}$$

Substituting in C_1 and C_2 in A.7 and setting $r = R$ makes

$$\Delta T = T_R + \frac{2T_R e^{-m'R}}{(m'R)^2}\left[\tanh(m'R) - 1\right] + \frac{2T_R}{m'R}\left[\frac{1}{m'R} - \tanh(m'R)\right]$$

Dimensionalizing results in

$$\theta^* = \theta(t)\left[1 + \frac{2e^{-m'R}}{(m'R)^2}\left[\tanh(m'R) - 1\right] + \frac{2}{m'R}\left[\frac{1}{m'R} - \tanh(m'R)\right]\right] \tag{A.8}$$

with θ^* equal to the actual temperature ratio at the tip of the fin. $\theta(t)$ is the temperature ratio calculated from the analytical solution of Fourier's heat conduction equation.

If $m'R > 100$, then A.8 reduces to

$$\theta^* = \theta(t)\left[1 + \frac{2}{m'R}\left(\frac{1}{m'R} - 1\right)\right] \tag{A.9}$$

The sensitivity coefficients of A.8 and A.9 are:

$$\frac{d\theta^*}{dm'} = \theta(t)\left[\frac{2e^{-m'R}}{(m'R)^2}\left(\frac{2}{m'} + R\right)\left(1 - \tanh(m'R)\right) + \frac{2}{m'R}\left(\frac{1}{m'}\tanh(m'R) - \frac{2}{(m')^2R} - R\operatorname{sech}^2(m'R)\right)\right] \tag{A.10}$$

for $m'R > 100$

$$\frac{d\theta^*}{dm'} = \theta(t)\left[\frac{2}{(m')^2R}\left(1 - \frac{2}{m'R}\right)\right] \tag{A.11}$$

APPENDIX B

Results of estimating diffusivity for 2% KELSET-water solutions and for three different can sizes.

- α_1 - diffusivity estimated using equations 3 and 6
- α_2, m' - diffusivity and probe factor estimated using equations 3, 6, and 12
- α_3 - diffusivity estimated from f_h (equation 10)
- MSE - is the mean square error of the estimates

* - denotes values that were not used in the calculation of the mean and standard deviation of the estimate.

° - denotes f_h values that were not calculated by successive iteration, but by regressing the data having a temperature ratio $<$ 0.55.

303x406 Can

Run #	α_1 x10^3 (m^2/hr)	MSE (°C)	α_2 x10^3 (m^2/hr)	m´ (m^{-1})	MSE (°C)	f_h (hr)	α_3 x10^3 (m^2/hr)
1	.6067	.0828	.6057	24701*	.0827	.7268°	.6549
2	.6098	.0302	.6098	∞*	.03086	.7727°	.6160
3	.6109	.1195	.6109	∞*	.1219	.7477°	.6366
4	.5919	.0695	.5919	∞*	.0709	.7979°	.5966
5	.5930	.0253	.5930	∞*	.0258	.8062°	.5904
6	.5992	.0625	.5938	4706	.00902	.8108°	.5870
7	.6044	.0333	.6008	6945	.01035	.8002°	.5948
8	.6032	.1197	.5951	3131	.00301	.8137°	.5840
9	.6008	.0809	.5941	3797	.00467	.8101°	.5876
10	.6016	.0368	.5974	6010	.00553	.8091°	.5883
11	.5983	.0260	.5958	9825*	.0159	.8089	.5884
12	.6100	.0469	.6062	6786	.0245	.7777°	.6120
13	.6052	.0376	.6030	11554*	.0299	.7774°	.6123
14	.6055	.0471	.6009	5619	.0131	.7961°	.5979
15	.6117	.0982	.6117	∞*	.1002	.7387°	.6443
16	.5975	.0436	.5975	∞*	.0445	.7819	.6098
17	.6041	.0693	.5984	4454	.0137	.7965	.5976
18	.6017	.0575	.5970	5460	.0216	.7964	.5977
19	.6016	.0721	.5968	5337	.0331	.8009	.5943
20	.5998	.0429	.5955	5904	.0107	.8054	.5910
21	.6010	.0507	.5967	5894	.0184	.7964	.5976
22	.6000	.0693	.5941	4276	.0096	.8068	.5899
23	.6014	.0738	.5954	4229	.0118	.7962	.5978
24	.6015	.0958	.5947	3703	.0159	.8065	.5902
25	.5978	.0887	.5911	3770	.0100	.8180	.5819
$\bar{x}$	.6023	.0632	.5987	5001	.0295	.7920	.6016
$S_{\bar{x}}$	.005024	.0274	.005947	1153	.0313	.0237	.0188

303x406 Can

Run #	$\alpha_2-\alpha_1$ x10^3 (m^2/hr)	% Diff. $(\alpha_2-\alpha_1)/\alpha_2$	$\alpha_2-\alpha_3$ x10^3 (m^2/hr)	% Diff. $(\alpha_2-\alpha_3)/\alpha_2$
1	-.001	-.165	-.0492	-8.12
2	0	0	-.0062	-1.02
3	0	0	-.0257	-4.21
4	0	0	-.0047	-.794
5	0	0	.0026	.438
6	-.0054	-.909	.0068	1.15
7	-.0036	-.599	.0060	.999
8	-.0081	-1.36	.0111	1.87
9	-.0067	-1.13	.0065	1.09
10	-.0042	-.703	.0091	1.52
11	-.0025	-.420	.0074	1.24
12	-.0038	-.627	-.0058	-.957
13	-.0022	-.365	-.0093	-1.54
14	-.0046	-.765	.0030	.500
15	0	0	-.0326	-5.33
16	0	0	-.0123	-2.06
17	-.0057	-.953	.0008	.134
18	-.0047	-.787	-.0007	-.117
19	-.0048	-.804	.0025	.419
20	-.0043	-.722	.0045	.756
21	-.0043	-.720	-.0009	-.151
22	-.0059	-.993	.0042	.707
23	-.0060	-1.01	-.0024	-.403
24	.0068	-1.14	.0045	.757
25	-.0067	-1.13	.0092	1.56
$\bar{x}$	-.0037	-.612	-.0029	-.463
$S_{\bar{x}}$	.0026	.436	.0142	2.34

307x409 Can

Run #	α_1 x10^3 (m^2/hr)	MSE (°C)	α_2 x10^3 (m^2/hr)	m´ (m^{-1})	MSE (°C)	f_h (hr)	α_3 x10^3 (m^2/hr)
1	.6071	.2694	.5944	1831	.000836	.9583	.5830
2	.6019	.1355	.5926	2491	.002262	.9658	.5785
3	.6145	.3602	.5997	1591	.000818	.9324	.5992
4	.6063	.3817	.5920	1630	.00183	.9521	.5868
5	.6041	.3223	.5909	1772	.00628	.9621	.5807
6	.6000	.2692	.5872	1780	.00601	.9807	.5697
7	.6040	.3095	.5904	1711	.00358	.9711	.5753
8	.6116	.1091	.6040	3098	.0167	.8941°	.6251
9	.6054	.2488	.5934	1956	.00451	.9270°	.6029
10	.6111	.4789	.5941	1377	.00253	.9672	.5777
11	.6117	.3195	.5977	1682	.000305	.9615	.5811
12	.6063	.2081	.5952	2090	.00202	.9221	.6059
13	.6080	.2361	.5960	1946	.000655	.9223	.6057
14	.6133	.1743	.6029	2266	.00221	.9153	.6104
15	.6135	.4001	.5977	1489	.000458	.9254	.6038
16	.6274	1.037	.6025	971.2	.00348	.9163	.6097
17	.6287	1.136	.6023	915.6	.002487	.8941	.6249
18	.6114	.2641	.5990	1890.9	.003776	.9009	.6201
19	.6062	.1423	.5972	2602	.00259	.9135	.6116
20	.6167	.2485	.6042	1890	.00168	.8873	.6297
21	.6075	.1957	.5969	2196	.00286	.8945	.6246
22	.6099	.2060	.5966	1764	.000297	.9228	.6054
23	.6157	.3549	.6007	1566	.002145	.9354	.5975
24	.6133	.1381	.6042	2593	.002218	.9058	.6170
25	.6115	.2227	.5998	2011	.00106	.9362°	.5970
$\bar{x}$	.6107	.3267	.5973	1884	.00294	.9306	.6009
$S_{\bar{x}}$	.006774	.2464	.004705	488.1	.00328	.0276	.01775

307x409 Can

Run #	$\alpha_2-\alpha_1$ x10³ (m²/hr)	% Diff. $(\alpha_2-\alpha_1)/\alpha_2$	$\alpha_2-\alpha_3$ x10³ (m²/hr)	% Diff. $(\alpha_2-\alpha_3)/\alpha_2$
1	-.0127	-2.14	.0114	1.92
2	-.0093	-1.57	.0141	2.38
3	-.0148	-2.47	.0005	.0834
4	-.0143	-2.42	.0052	.878
5	-.0132	-2.23	.0102	1.73
6	-.0128	-2.18	.0175	2.98
7	-.0136	-2.30	.0151	2.56
8	-.0076	-1.26	-.0211	-3.49
9	-.012	-2.02	-.0095	-1.60
10	-.017	-2.86	.0164	2.76
11	-.014	-2.34	.0166	2.78
12	-.0111	-1.87	-.0107	-1.80
13	-.012	-2.01	-.0097	-1.63
14	-.0104	-1.73	-.0075	-1.24
15	-.0158	-2.64	-.0061	-1.02
16	-.0249	-4.13	-.0072	-1.19
17	-.0264	-4.38	-.0226	-3.75
18	-.0124	-2.07	-.0211	-3.52
19	-.009	-1.51	-.0144	-2.41
20	-.0125	-2.07	-.0255	-4.22
21	-.0106	-1.78	-.0277	-4.64
22	-.0133	-2.23	-.0088	-1.47
23	-.015	-2.50	.0032	.533
24	-.0091	-1.51	-.0128	-2.12
25	-.0117	-1.95	.0028	.467
$\bar{x}$	-.0134	-2.25	-.00367	-.603
$S_{\bar{x}}$	.00431	.715	.0143	2.400

401x411 Can

Run #	α_1 x10^3 (m^2/hr)	MSE (°C)	α_2 x10^3 (m^2/hr)	m' (m^{-1})	MSE (°C)	f_h (hr)	α_3 x10^3 (m^2/hr)
1	.5949	.03108	.5911	5296	.00585	1.168	.6299
2	.5984	.0528	.5931	6809	.00557	1.163	.6323
3	.6026	.1859	.5929	3133	.0194	1.176°	.6253
4	.5961	.0389	.5921	5368	.0132	1.185°	.6206
5	.5986	.1242	.5903	4258	.00169	1.267°	.5803
6	.5880	.02348	.5844	5176	.00109	1.277	.5760
7	.5921	.01254	.5896	7526	.00289	1.238	.5942
8	.6040	.2023	.5930	1741	.000386	1.221	.6024
9	.6009	.0547	.5952	3555	.00348	1.209	.6086
10	.5985	.04117	.5936	5915	.00402	1.210	.6078
11	.5993	.2235	.5877	1656	.00223	1.261	.5835
12	.5960	.07614	.5892	2762	.000839	1.241	.5927
13	.5986	.09646	.5908	2424	.00100	1.222	.6021
14	.5982	.04891	.5927	3459	.00110	1.232	.5971
15	.6003	.01544	.6000	59080*	.0155	1.156	.6365
16	.6080	.1114	.6008	∞*	.0260	1.147	.6416
17	.5989	.1177	.5907	2311	.0114	1.164	.6320
18	.5955	.1382	.5955	∞*	.140	1.078	.6825
19	.5933	.0339	.5889	4297	.00134	1.231	.5972
20	.5936	.04043	.5890	4031	.00145	1.219	.6033
21	.6068	.4574	.5915	11810*	.00377	1.207	.6092
22	.5935	.1114	.5856	2594	.000599	1.222	.6016
23	.5999	.1283	.5913	2366	.00106	1.241	.5928
24	.5989	.00533	.5985	56960*	.00521	1.190	.6179
25	.5959	.0955	.5886	2598	.000526	1.228	.5989
$\bar{x}$	.5980	.0987	.5918	3864	.01078	1.206	.6106
$S_{\bar{x}}$	.004481	.0960	.00398	1686	.0277	.044	.0233

401x411 Can

Run #	$\alpha_2 - \alpha_1$ x10^3 (m^2/hr)	% Diff. $(\alpha_2 - \alpha_1)/\alpha_2$	$\alpha_2 - \alpha_3$ x10^3 (m^2/hr)	% Diff. $(\alpha_2 - \alpha_3)/\alpha_2$
1	-.0038	-.643	-.0388	-6.56
2	-.0053	-.894	-.0392	-6.61
3	-.0097	-1.64	-.0324	-5.47
4	-.0040	-.674	-.0285	-4.81
5	-.0083	-1.41	.0100	1.69
6	-.0036	-.616	.0084	1.44
7	-.0025	-.424	-.0046	-.780
8	-.0110	-1.85	-.0094	-1.59
9	-.0057	-.958	-.0134	-2.25
10	-.0049	-.825	-.0142	-2.39
11	-.0116	-1.97	.0042	.715
12	-.0068	-1.15	-.0035	-.594
13	-.0078	-1.32	-.0113	-1.91
14	-.0055	-.928	-.0044	-.742
15	-.0003	-.050	-.0365	-6.08
16	-.0072	-1.20	-.0408	-6.79
17	-.0082	-1.39	-.0413	-6.99
18	0	0	-.0870	-14.6
19	-.0044	-.747	-.0083	-1.41
20	-.0046	-.781	-.0143	-2.43
21	-.0153	-2.59	-.0177	-2.99
22	-.0079	-1.35	-.0160	-2.73
23	-.0086	-1.45	-.0015	-.254
24	-.0004	-.0668	-.0194	-3.24
25	-.0073	-1.24	-.0103	-1.75
$\bar{x}$	-.0062	-1.05	-.0188	-3.17
$S_{\bar{x}}$	.00363	.614	.0209	3.51

APPENDIX C

Results of estimating diffusivity for different food products in a 307x409 can.

α_1 - diffusivity estimated using equations 3 and 6

α_2 - diffusivity estimated using equations 3, 6, and 12 with $m' = 1900\ m^{-1}$ - the average value of m' from the 307x409 results in Appendix A

α_3 - diffusivity estimated from f_h (equation 10)

MSE - the mean square error of the estimate

Products with the same number were processed, allowed to equilibrate to room temperature, and reprocessed.

Product	α_1 x10^3 (m^2/hr)	MSE (°C)	α_2 (m'=1900) x10^3 (m^2/hr)	MSE (°C)	f_h (hr)	α_3 x10^3 (m^2/hr)
Pumpkin[1]	.5902	.2774	.5780	.1220	.8210	.6702
Pumpkin[2]	.5905	.2892	.5782	.1047	.8215	.6698
Pumpkin[3]	.5817	.0872	.5698	.06377	.9674	.5688
Pumpkin[4]	.5901	.4059	.5781	.9664	.7958	.6915
Pumpkin[5]	.5782	.2151	.5664	.00549	.9760	.5638
Pumpkin[6]	.5799	.3314	.5681	.00415	.9875	.5572
Pumpkin[7]	.5866	.1140	.5747	.03825	.9592	.5736
Pumpkin[8]	.5891	.1144	.5772	.03405	.9561	.5755
Pumpkin[9]	.5835	.1814	.5717	.00815	.9727	.5657
Pumpkin[10]	.5829	.2434	.5711	.00068	.9753	.5642
Lima Bean Puree[1]	.5833	.1748	.5715	.00718	1.003	.5571
Lima Bean Puree[2]	.5818	.2379	.5700	.00316	.9859	.5670
Lima Bean Puree[1]	.5828	.2480	.5710	.00106	.9956	.5614
Lima Bean Puree[2]	.5823	.3128	.5705	.00282	.9857	.5670
Mayonnaise[1]	.4104	14.99	.4007	10.375	1.782	.3136
Mayonnaise[2]	.4168	16.53	.4070	11.562	1.759	.3178
Mayonnaise[1]	.4022	16.59	.3933	11.920	1.769	.3158
Mayonnaise[3]	.4112	14.57	.4022	10.280	1.707	.3275
Baked Beans[1]	.5647	.4652	.5532	.1229	.9709	.5757
Baked Beans[2]	.5657	.5574	.5540	.1528	.9340	.5984
Baked Beans[1]	.5522	.5623	.5410	.0583	1.067	.5236
Baked Beans[2]	.5568	.6770	.5455	.09628	1.036	.5393
Baked Beans[3]	.5627	.9054	.5512	.168	1.057	.5286
Potato Salad[1]	.5594	.9054	.5481	.03668	1.035	.5399
Potato Salad[1]	.5559	.4543	.5446	.02837	1.059	.5276
Potato Salad[2]	.5618	.3923	.5504	.01794	1.019	.5486

Product	$\alpha_2-\alpha_1$ x10^3 (m^2/hr)	% Diff. $(\alpha_2-\alpha_1)/\alpha_2$	$\alpha_2-\alpha_3$ x10^3 (m^2/hr)	% Diff. $(\alpha_2-\alpha_3)/\alpha_2$
Pumpkin[1]	-.0122	-2.11	-.0922	-15.9
Pumpkin[2]	-.0123	-2.13	-.0916	-15.8
Pumpkin[3]	-.0119	-2.09	.0010	.175
Pumpkin[4]	-.0120	-2.08	-.1134	-19.6
Pumpkin[5]	-.0118	-2.08	.0026	.459
Pumpkin[6]	-.0118	-2.08	.0109	1.92
Pumpkin[7]	-.0119	-2.07	.0011	.191
Pumpkin[8]	-.0119	-2.06	.0017	.294
Pumpkin[9]	-.0118	-2.06	.0060	1.05
Pumpkin[10]	-.0118	-2.07	.0069	1.21
Lima Bean Puree[1]	-.0118	-2.06	.0144	2.52
Lima Bean Puree[2]	-.0118	-2.07	.0030	.526
Lima Bean Puree[1]	-.0118	-2.07	.0096	1.68
Lima Bean Puree[2]	-.0118	-2.07	.0035	.613
Mayonnaise[1]	-.0097	-2.42	.0871	21.7
Mayonnaise[2]	-.0098	-2.41	.0892	21.9
Mayonnaise[1]	-.0089	-2.26	.0775	19.7
Mayonnaise[3]	-.0090	-2.24	.0747	18.6
Baked Beans[1]	-.0115	-2.08	-.0225	-4.07
Baked Beans[2]	-.0117	-2.11	-.0444	-8.01
Baked Beans[1]	-.0112	-2.07	.0174	3.22
Baked Beans[2]	-.0113	-2.07	.0062	1.14
Baked Beans[3]	-.0115	-2.09	.0226	4.10
Potato Salad[1]	-.0113	-2.06	.0082	1.50
Potato Salad[1]	-.0113	-2.07	.0170	3.12
Potato Salad[2]	-.0114	-2.07	.0018	.327

Product	α_1 x10^3 (m^2/hr)	MSE (°C)	α_2 (m' =1900) x10^3 (m^2/hr)	MSE (°C)	f_h (hr)	α_3 x10^3 (m^2/hr)
Apple Sauce[1]	.5784	.8232	.5667	.1445	1.019	.5483
Apple Sauce[2]	.5756	.6530	.5639	.01775	.9849	.5675
Apple Sauce[3]	.5642	.4303	.5529	.02411	1.050	.5321
Tomato Paste[1]	.5613	.5416	.5500	.05027	1.035	.5398
Tomato Paste[1]	.5557	.5042	.5445	.03935	1.021	.5474
Tomato Paste[2]	.5532	.5885	.5420	.06130	1.023	.5466
Baby Food-Apricot[1]	.5723	.2817	.5608	.00337	1.019	.5483
Baby Food-Apricot[2]	1.076	46.28	1.054	42.95	.9599	.5822
Baby Food-Apricot[1]	.5683	.2265	.5569	.00764	1.015	.5508
Mashed Potatoes[1]	.5773	.3604	.5655	.0425	.950	.5883
Mashed Potatoes[1]	.5900	.4033	.5778	.1898	.904	.6183
Mashed Potatoes[1]	.5920	.1756	.5801	.05244	.9476	.5898
Mashed Potatoes[2]	.5661	.6646	.5545	.1415	.9882	.5656
Mashed Potatoes[2]	.6064	.3179	.5941	.00959	.9203	.6073
Mashed Potatoes[2]	.6015	.4163	.5893	.01498	.9581	.5833
Mashed Potatoes[3]	.5918	.3097	.5799	.00406	.9927	.5631
Mashed Potatoes[3]	.5908	.2736	.5788	.00301	.9947	.3619
Mashed Potatoes[3]	.5887	.4320	.5769	.02586	1.004	.5567
Mashed Potatoes[3]	.5886	.3765	.5768	.01094	.9864	.5666
Pea Puree[1]	.5923	.6287	.5802	.07130	.9940	.5623
Pea Puree[2]	.5954	.5001	.5832	.03485	.9870	.5663
Pea Puree[1]	.5883	.5474	.5765	.05567	.9979	.5601
Pea Puree[2]	.5851	.4336	.5733	.02189	.9934	.5627

Product	$\alpha_2-\alpha_1$ x10^3 (m^2/hr)	% Diff. $(\alpha_2-\alpha_1)/\alpha_2$	$\alpha_2-\alpha_3$ x10^3 (m^2/hr)	% Diff. $(\alpha_2-\alpha_3)/\alpha_2$
Apple Sauce[1]	-.0117	-2.07	.0184	3.25
Apple Sauce[2]	-.0117	-2.07	-.0036	-.638
Apple Sauce[3]	-.0113	-2.04	-.0208	3.76
Tomato Paste[1]	-.0113	-2.05	.0102	1.85
Tomato Paste[1]	-.0112	-2.06	-.0029	-.533
Tomato Paste[2]	-.0112	-2.07	-.0046	-.849
Baby Food-Apricot[1]	-.0115	-2.05	.0125	2.23
Baby Food-Apricot[2]	-.0220	-2.09	.4718	44.8
Baby Food-Apricot[1]	-.0114	-2.05	.0061	1.09
Mashed Potatoes[1]	-.0118	-2.09	-.0228	-4.03
Mashed Potatoes[1]	-.0122	-2.11	-.0405	-7.01
Mashed Potatoes[1]	-.0119	-2.05	-.0097	-1.67
Mashed Potatoes[2]	-.0116	-2.09	-.0111	-2.00
Mashed Potatoes[2]	-.0123	-2.07	-.0132	-2.22
Mashed Potatoes[2]	-.0122	-2.07	.0060	1.02
Mashed Potatoes[3]	-.0119	-2.05	.0168	2.90
Mashed Potatoes[3]	-.0120	-2.07	.0169	2.92
Mashed Potatoes[3]	-.0118	-2.05	.0202	3.50
Mashed Potatoes[3]	-.0118	-2.05	.0102	1.77
Pea Puree[1]	-.0121	-2.09	.0179	3.09
Pea Puree[2]	-.0122	-2.09	.0169	2.90
Pea Puree[1]	-.0118	-2.05	.0164	2.85
Pea Puree[2]	-.0118	-2.06	.0106	1.85

Product	α_1 x10^3 (m^2/hr)	MSE (°C)	α_2 x10^3 (m^2/hr)	MSE (°C)	f_h (hr)	α_3 x10^3 (m^2/hr)
Pumpkin						
$\bar{x}$	.5853	.2259	.5733	.1338	.9234	.6000
$S_{\bar{x}}$	.00462	.1037	.00448	.2957	.0771	.0538
Lima Bean Puree						
$\bar{x}$	.5826	.2434	.5707	.00356	.9925	.5631
$S_{\bar{x}}$	.000645	.0565	.000645	.00259	.00836	.00481
Mayonnaise						
$\bar{x}$	.4101	15.67	.4008	11.03	1.754	.3187
$S_{\bar{x}}$	.00602	1.042	.00568	.830	.0329	.00613
Baked Beans						
$\bar{x}$	.5604	.6335	.5490	.1197	1.013	.5531
$S_{\bar{x}}$	.00575	.1696	.00556	.0440	.0579	.0325
Potato Salad						
$\bar{x}$	.5590	.4520	.5477	.02767	1.038	.5387
$S_{\bar{x}}$	.00297	.0586	.00292	.00939	.0201	.0106
Apple Sauce						
$\bar{x}$	.5727	.6355	.5612	.0621	1.018	.5493
$S_{\bar{x}}$	.00752	.1970	.0073	.0714	.0326	.0177

Product	$\alpha_2-\alpha_1$ x10^3 (m^2/hr)	$\alpha_2-\alpha_3$ x10^3 (m^2/hr)	% Diff. $(\alpha_2-\alpha_1)/\alpha_2$	% Diff. $(\alpha_2-\alpha_3)/\alpha_2$
Pumpkin				
$\bar{x}$	-.0119	-.0267	-2.083	-4.61
$S_{\bar{x}}$	.00018	.0504	.0212	8.72
Lima Bean Puree				
$\bar{x}$	-.0118	.00763	-2.067	1.335
$S_{\bar{x}}$	0	.00542	.00222	.948
Mayonnaise				
$\bar{x}$	-.0093	.0821	-2.333	20.49
$S_{\bar{x}}$	.00047	.0071	.0954	1.623
Baked Beans				
$\bar{x}$	-.0114	-.0041	-2.084	-.7256
$S_{\bar{x}}$	.00019	.0285	.0172	5.162
Potato Salad				
$\bar{x}$	-.0113	.0090	-2.069	1.648
$S_{\bar{x}}$	-.00006	.0076	.0067	1.403
Apple Sauce				
$\bar{x}$	-.0116	.0119	-2.061	2.124
$S_{\bar{x}}$	.00023	.0134	.0158	2.406

Product	α_1 x10^3 (m^2/hr)	MSE (°C)	α_2 x10^3 (m^2/hr)	MSE (°C)	f_h (hr)	α_3 x10^3 (m^2/hr)
Tomato Paste						
$\bar{x}$	.5567	.5448	.5455	.0503	1.026	.5446
$S_{\bar{x}}$	.00415	.0422	.00409	.0110	.0076	.00418
Mashed Potatoes						
$\bar{x}$	.5864	.3131	.5745	.0949	.9339	.5988
$S_{\bar{x}}$	.00797	.1210	.00785	.0823	.0259	.0169
Mashed Potatoes						
$\bar{x}$	.5880	.4663	.5793	.0554	.9556	.5854
$S_{\bar{x}}$	.02773	.1787	.0216	.0747	.0340	.0209
Mashed Potatoes						
$\bar{x}$	.5900	.3480	.5781	.01097	.9945	.5621
$S_{\bar{x}}$	.00158	.0704	.00151	.01053	.00728	.00410
Pea Puree						
$\bar{x}$	.5903	.5275	.5783	.0459	.9931	.5629
$S_{\bar{x}}$	.0045	.0821	.00432	.0219	.0045	.00257

Product	$\alpha_2-\alpha_1$ x10^3 (m^2/hr)	$\alpha_2-\alpha_3$ x10^3 (m^2/hr)	% Diff. $(\alpha_2-\alpha_1)/\alpha_2$	% Diff. $(\alpha_2-\alpha_3)/\alpha_2$
Tomato Paste				
$\bar{x}$	-.0112	.0009	-2.059	.1579
$S\bar{x}$	.00006	.0081	.0058	1.478
Mashed Potatoes				
$\bar{x}$	-.0100	-.0243	-2.083	-4.238
$S\bar{x}$	.00021	.0155	.0302	2.67
Mashed Potatoes				
$\bar{x}$	-.0120	-.0261	-2.077	-1.069
$S\bar{x}$	.00038	.0417	.0127	1.810
Mashed Potatoes				
$\bar{x}$	-.0119	.0160	-2.054	2.772
$S\bar{x}$	.000096	.00419	.0130	.725
Pea Puree				
$\bar{x}$	-.0120	.01545	-2.071	2.670
$S_{\bar{x}}$	.00021	.00330	.0215	.556

APPENDIX D

Results of estimating diffusivity from processes that have a long come-up time, for cans with a head space, and results for reprocessing of the same KELSET sample.

α_1 - diffusivity estimated using equations 3 and 6

α_2, m' - diffusivity and probe factor estimated using equations 3, 6, and 12

α_3 - diffusivity estimated from f_h (equation 10)

MSE - mean square error of estimate

Can Size	α_1 x10^3 (m^2/hr)	MSE (°C)	α_2 x10^3 (m^2/hr)	m' (m^{-1})	MSE (°C)	f_h (hr)	α_3 x10^3 (m^2/hr)
Head Space (1.27 cm)							
307x409							
1	.6020	.1186	.5936	2733	.00105	.9659	.5786
2	.6002	.1186	.5919	2754	.00441	.9662	.5785
401x411							
1	.5928	.0612	.5869	3120	.00309	1.297	.5670
2	.5930	.0306	.5888	4400	.000672	1.265	.5812
Come-up Time (8 min.)							
307x409							
1	.5625	.4883	.5625	∞	.4962	.9524	.5869
2	.5617	.8410	.5617	∞	.8550	.9424	.5931
2% KELSET							
307x409							
1	.5919	.00490	.6041	(m=1900)	.2009	.9653	.5790
2	.5948	.0253	.6070	(m=1900)	.1415	.9571	.5840
3	.5954	.0104	.6077	(m=1900)	.3766	.9711	.5755
4	.6221	1.471	.6348	(m=1900)	.9767	.8694	.6429