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A COMPREHENSIVE MODEL TO DETERMINE THE EFFECTS OF TEMPERATURE AND SPECIES FLUCTUATIONS ON REACTION RATES IN TURBULENT REACTING FLOWS*

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1. Introduction

1.1 Overview

The prediction of the behavior of turbulent reacting flows is a major concern of current combustion research. Such modeling is required in order to enhance the understanding of the phenomena involved and to design and evaluate the performance of combustion devices. A principal element to be derived from the modeling of these flows is an expression for the reaction rates of the various species involved in any particular combustion process under consideration.

Currently, several approaches for the determination of the properties of turbulent, reacting flows exist.[1] Of the present approaches, the method of utilizing an assumed probability density function (pdf) for temperature and species, concentrations has been selected for use in this study. The motivation for selecting this approach is its relative computational simplicity and its basis in the probabilistic nature of turbulence.

1.2 Objective

This work is examining the effects of temperature and species concentrations fluctuations on reaction rates in turbulent, reacting flows by means of the presumed pdf approach. The following items are the subject of the present study:

1. The utilization of the temperature-derived most-likely pdf of reference (2) to describe the effects of temperature fluctuations on the Arrhenius reaction rate constant.

2. The utilization of the most-likely bivariate pdf of reference (2) to describe effects of temperature and species concentrations fluctuations on the reaction rate.

3. Development of a criterion for the use of an "appropriate" temperature pdf.

Section 2 presents a brief review of the general theory of pdf's. Sections 3 and 4 review the formulation of models to calculate the mean turbulent Arrhenius reaction rate constant and the mean turbulent reaction rate, respectively. Section 5 presents the results of calculations using these models. Section 6 presents conclusions and the direction of future work, dealing with the combined effects of temperature and species fluctuations on reaction rates. In Section 7, we deal with the criterion for the selection of a temperature pdf.

2. Review of the General Theory

The discussion in this section is taken largely from reference (1).

2.1 Probability Density Functions

A parameter x is said to be a continuous random variable if there exists a probability density function, p(x), which satisfied the following conditions.[3]

$$p(x) \geq 0 \quad \text{for all } x \tag{1a}$$

$$\int_{-\infty}^{\infty} p(x)\,dx = 1 \tag{1b}$$

The pdf may, of course, be defined on an interval other than $(-\infty, +\infty)$, for example $(0,1)$. Since the pdf is defined on a specific interval, the functional value of $p(x)$ is zero elsewhere.

Equation (1) must be satisfied by a pdf of a one-dimensional continuous random variable. Probability density functions may be written for a multi-dimensional continuous random variable. A probability density function for a two-dimensional continuous random variable, denoted $p(x,y)$, is termed a bivariate or joint pdf. For such a pdf, the conditions corresponding to equation (1) are:

$$p(x,y) \geq 0 \qquad \text{for all } x \text{ and } y \tag{2a}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p(x,y)\,dx\,dy = 1 \tag{2b}$$

The expected, or mean value of a one-dimensional continuous random variable, x, is expressed as:

$$\mu_x = E(x) = \int_{-\infty}^{\infty} x \cdot p(x)\,dx \tag{3}$$

The variance of a one-dimensional continuous random variable, x, is expressed as:

$$\sigma_x^2 = V(x) = \int_{-\infty}^{\infty} (x - E(x))^2 \cdot p(x)\,dx \tag{4}$$

A useful quantity derived from the variance is the standard deviation which is the square root of the variance. Equation (4) is a special case of the more general expression for the Kth moment of a random variable, x, about its expectation. The general expression for the Kth moment of a random variable is given by [3]:

$$\mu_K = \int_{-\infty}^{\infty} (x - E(x))^K \cdot p(x)\, dx \quad \text{for } K = 2, 3, 4, \ldots \tag{5}$$

Clearly, for the special case of K=2, equation (5) is equal to equation (4).

Equation (3) may be extended to functions of a continuous random variable. In the case of a function f(x) of a one-dimensional random variable having a pdf p(x), the mean value of f(x) is:

$$\overline{f(x)} = \int_{-\infty}^{\infty} f(x) \cdot p(x)\, dx \tag{6}$$

Similarly, in the case of a function g(x,y) of a two-dimensional random variable, having the joint pdf p(x,y), the mean value of g(x,y) is:

$$\overline{g(x,y)} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x,y) \cdot p(x,y)\, dx\, dy \tag{7}$$

The correlation coefficient, ρ_{xy}, is a parameter defined with respect to the two-dimensional/continuous random variable (x,y) and is expressed as:

$$\rho_{xy} = \frac{E\{[x-E(x)][y-E(y)]\}}{\sqrt{V(x)\,V(y)}} \tag{8}$$

The correlation coefficient is a measure of the degree of linearity between x and y. Values of the correlation coefficient near +1 or -1 reflect a high degree of linearity, while values of the correlation coefficient near zero indicate a lack of linearity. Positive values of the correlation coefficient indicate that as y increases, x increases. Negative values of the correlation coefficient indicate that y increases as x decreases.

The numerator of equation (8) is defined as the covariance of x and y. The covariance is denoted by σ_{xy} and is expressed as:

$$\sigma_{xy} = \overline{x'y'} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (x-\bar{x})(y-\bar{y})\cdot p(x,y)\,dx\,dy \tag{9}$$

The significance of the covariance can be ascertained by considering a two-dimensional random variable (x,y). x and y are termed independent random variables if the value of x has no influence on the value of y (and likewise, the value of y has no influence on the value of x). When x and y are independent random variables the covariance is zero. Hence, the covariance may be considered as a minimum "criterion" of statistical dependence. This criterion can assure, at the very least, that when the covariance is not zero, the variables are not independent. However, no statement can be made concerning independence on this basis alone, if the covariance is zero.

2.2 Arrhenius Reaction Rate Constant and Reaction Rate Expressions

For the purposes of the study presented herein, the following one-step, irreversible reaction is considered:

$$F + \nu O \rightarrow P \tag{10}$$

F, O, P = fuel oxidizer, and product species respectively

ν = stoichiometric coefficient

The disappearance of F and O are related by:

$$-\frac{dc_F}{dt} = -\frac{1}{\nu}\frac{dc_O}{dt} \tag{11}$$

where: c_F, c_O = concentrations of fuel and oxidizer, respectively

The negative signs in equation (11) indicate that the concentrations of F and O decrease as the reaction proceeds. The reaction rate of fuel is expressed as:

$$\dot{w}_F = -\frac{dc_F}{dt} = K(T)\, c_F^{\,n}\, c_O^{\,m} \tag{12}$$

where k(T) = Arrhenius reaction rate constant

T = temperature

n, m = constants dependent upon the particular reaction.

The Arrhenius reaction rate constant is expressed as:

$$k(T) = AT^B \exp(-T_A/T) \tag{13}$$

where A, B = constants dependent upon the particular reaction

T_A = activation temperature of the particular reaction.

Equation (13) can be modified by the introduction of the dimensionless temperature:

$$t = \frac{T - Tmin}{Tmax - Tmin} \tag{14}$$

The temperatures Tmax and Tmin are defined so that the dimensionless temperature t can only assume values within the interval (0,1). Thus, Tmin may be the lowest temperature of the unreacted constituents and Tmax may be the equilibrium combustion temperature of the reaction. Substitution of (14) into (13) yields:

$$K(t) = A\left(k_1 t + k_2\right)^B \cdot \exp\left[-T_A/(k_1 t + k_2)\right] \tag{15}$$

where k_1 = Tmax - Tmin

k_2 = Tmin

Equation (12) is also modified by the introduction of the following dimensionless concentrations:

$$r_F = \frac{c_F - c_F^{min}}{c_F^{max} - c_F^{min}} \quad , \quad r_0 = \frac{c_0 - c_0^{min}}{c_0^{max} - c_0^{min}} \tag{16}$$

In these expressions, "max" and "min" denote maximum and minimum values, respectively. Equation (16) ensures that r_F and r_0 only assume values within the interval (0,1). For the case where the minimum concentrations are zero and the maximum concentrations are the initial values, the combination of equations (12) and (16) yields:

$$\dot{w}_F = K(t)\left(r_F c_F^{\circ}\right)^n \left(r_o c_o^{\circ}\right)^m \tag{17}$$

where c_F°, c_0° = initial concentrations of fuel and oxidizer, respectively

2.3 Mean Turbulent Arrhenius Reaction Rate Constant and Mean Turbulent Reaction Rate Expressions

In a turbulent reacting flow, the mean turbulent Arrhenius reaction rate constant can be calculated by treating the temperature as a continuous random variable and specifying an appropriate probability density function for the temperature. This concept is employed in Reference (1) along with the analogs of equations (6) and (15) in the present work to yield:

$$\overline{K(t)} = \int_0^1 K(t) \cdot p(t)\, dt \tag{18}$$

where: $\overline{K(t)}$ = mean turbulent Arrhenius reaction rate constant.

The above expression provides a direct, relatively simple method of taking into account the effects of temperature fluctuations on the Arrhenius reaction rate constant in a turbulent, reacting flow.

Similarly, the expression for the mean turbulent reaction rate can be developed from an extension and combination of equations (7) and (17). Thus:

$$\overline{\dot{w}_F} = \int_0^1 \int_0^1 \int_0^1 \dot{w}_F \cdot p\left(t, r_F, r_o\right) dt\, dr_F\, dr_o \tag{19}$$

where $\overline{\dot{w}_F}$ = mean turbulent reaction rate of fuel.

This expression utilizes a joint pdf for temperature and species. Equations (18) and (19) can be applied to one-step reactions, or multi-step mechanisms, by considering each elementary reaction separately. The pdf's used here are considered to be valid at an instant in time, and thus are not functions of time.

In order to compare the magnitude of a mean turbulent Arrhenius reaction rate constant to the corresponding laminar term, an amplification ratio is defined. The laminar Arrhenius reaction rate constant is calculated by inserting the mean dimensionless temperature in equation (15). The amplification ratio is obtained by dividing equation (18) by (15):

$$Z = \overline{k_t}/k_\ell \tag{20}$$

where: Z = reaction rate constant amplification ratio

$\overline{k_t}$ = mean turbulent reaction rate constant

k_ℓ = corresponding "laminar" reaction rate constant

A similar term may be defined for the ratio of a mean turbulent reaction rate to the corresponding "laminar" reaction rate. The "laminar" reaction rate is calculated by inserting mean values of dimensionless temperature and concentrations into equation (17). The ratio of equation (19) to (17) defines the reaction rate amplification ratio:

$$Z' = \overline{\dot{w}} / \dot{w}_\ell \tag{21}$$

where Z' = reaction rate amplification ratio

$\overline{\dot{w}_t}$ = mean turbulent reaction rate

$\dot{w}_\ell$ = corresponding "laminar" reaction rate

Equation (21) is the reaction rate amplification ratio in which the mean turbulent reaction rate is calculated with consideration of the combined effects of temperature and species concentrations fluctuations. In order to compare this amplification ratio to one which considers only temperature fluctuations, the following is defined with the aid of equation (17):

$$Z' = \frac{\bar{K}_t \left(\bar{r}_F c_F^{\circ}\right)^n \left(\bar{r}_o c_o^{\circ}\right)^m}{K_\ell \left(\bar{r}_F c_F^{\circ}\right)^n \left(\bar{r}_o c_o^{\circ}\right)^m}$$

This expression involves a mean turbulent reaction rate in which a mean turbulent reacton rate constant is employed along with laminar values of concentrations. The corresponding laminar reaction rate also contains these same concentration terms. Thus, the concentration terms cancel. The reaction rate amplification ratio for this case is:

$$Z' = \frac{\bar{K}_t}{K_\ell} \qquad (22)$$

This amplification ratio may be compared to that calculated by use of equation (21). Hence, the combined effects of temperature and species concentrations fluctuations on the reaction rate may be compared to effects of only temperature fluctuations.

3. Probability Density Functions for Temperature

3.1 Most - Likely pdf

The most-likely pdf is shown in reference [2] to be the statistically-most-likely pdf of a continuous random variable for a given flow. It is important to note that although this pdf is the most-likely pdf, it is not necessarily the pdf for a given flow. The utility of the most-likely pdf is that any number of moments can be incorporated into the pdf and, hence, greater accuracy achieved.

Two possible shapes of the most-likely pdf for one variable (e.g., temperature) are shown in Figure 1

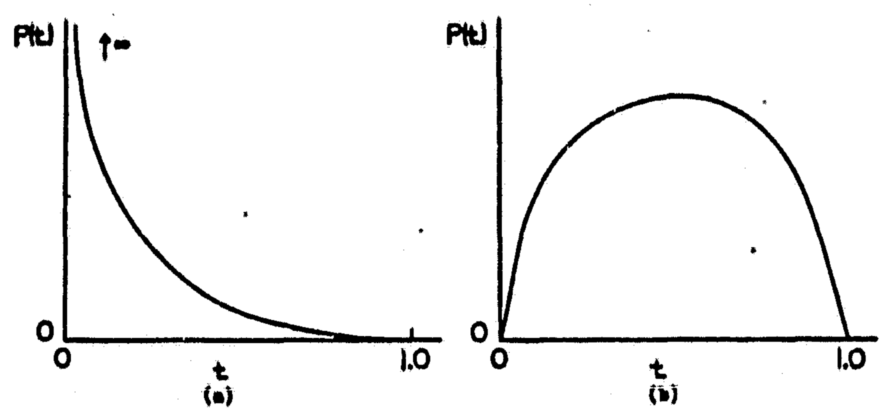

Figure 1. Possible shapes of the one-variable most-likely pdf (a) spike (b) Gaussian-like.

The expression for the temperature-derived most-likely pdf is:

$$p(t) = \exp\left[\lambda_0 + \lambda_1 t + \lambda_2 t^2\right] \tag{23}$$

where the constant coefficients $\lambda 0$, $\lambda 1$, $\lambda 2$ are obtained from the simultaneous solution of the following constraint equations for known values of dimension-less mean temperature and the mean square fluctuation of dimensionless temperature:

$$\int_0^1 p(t)\,dt = 1 \tag{24}$$

$$\int_0^1 t \cdot p(t)\,dt = \bar{t} \tag{25}$$

$$\int_0^1 (t-\bar{t})^2 \cdot p(t)\,dt = \overline{t'^2} \tag{26}$$

Equation (23) may be utilized in equation (18) to obtain the following expression for the mean turbulent reaction rate constant:

$$\bar{K}_t = A \int_0^1 (K_1 t + K_2)^B \cdot \exp\left[-T_A / (K_1 t + K_2)\right] \cdot p(t)\,dt \tag{27}$$

where p(t) is the temperature-derived most-likely pdf, equation (23).

The corresponding "laminar" term is calculated by use of $\bar{t}$ in equation (15). This yields:

$$K_\ell = A\,(K_1 \bar{t} + K_2)^B \cdot \exp\left[-T_A / (K_1 \bar{t} + K_2)\right] \tag{28}$$

The ratio of (27) to (28) is the reaction rate amplification ratio, Z:

$$Z = \bar{K}_t / K_\ell \tag{29}$$

For the purposes of a parameter study, values of mean temperature and mean square temperature fluctuation are selected in order to examine the effects of their variation on the mean turbulent Arrhenius reaction rate constant. The results of this study are presented in Section 5.

The computational procedure to determine the values of the reaction rate constant amplification ratio is described below:

Procedure:

1. Select values for A, B, TA, Tmin, Tmax, $\bar{t}$ and $\overline{t'^2}$
2. Utilize Newton's Method to solve for the constant coefficients of equation (23).
3. Numerically integrate equation (27) to obtain $\bar{K}_t$.
4. Utilize $\bar{t}$ in equation (28) to obtain $k\ell$
5. Calculate Z with equation (29).

3.2 Beta pdf

The beta pdf is utilized in Reference (1) as a pdf for the temperature. The selection of the beta pdf is based on its usefulness in approximating experimentally determined temperature pdf's in turbulent, non-reacting flows. Two possible shapes of the beta pdf are shown in Figure 2.

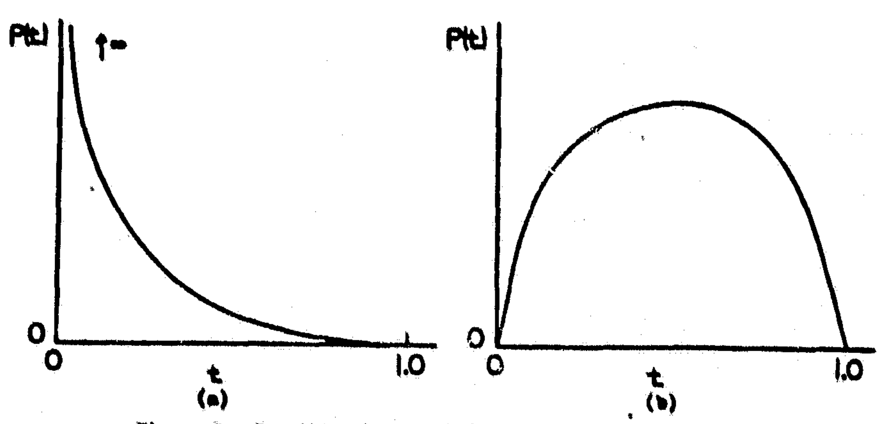

Figure 2. Possible shapes of the beta pdf: (a) resembling a spike, (b) Gaussian-like

The expression for the beta pdf is:

$$p(t) = \frac{\Gamma(a+b)}{\Gamma(a) + \Gamma(b)} \cdot t^{a-1} (1-t)^{b-1} \; ; \; 0 \leq t \leq 1 \tag{30}$$

where Γ = gamma function

a, b = constants dependent on $\bar{t}$ and $\overline{t'^2}$

The expressions for a and b are:

$$a = \bar{t} \left[\bar{t}(1-\bar{t})/\overline{t'^2} - 1 \right] \tag{31a}$$

$$b = (1-\bar{t}) \left[\bar{t}(1-\bar{t})/\overline{t'^2} - 1 \right] \tag{31b}$$

Equation (30 is utilized in equation (18) to obtain the following expression for the mean turbulent Arrhenius reaction rate constant:

$$\bar{K}_t = A \int_0^1 (K_1 t + K_2)^B \cdot \exp\left[-T_A / (K_1 t + K_2) \right] \cdot p(t) dt \tag{32}$$

where p(t) is the beta pdf.

The procedure for evaluating equation (32) is given in Reference (1). Equation (32) and equation (28) are inserted in Equation (29) to obtain the reaction rate constant amplification ratio.

The results of a parameter study with the model given by equation (32) are presented in Reference (1). In this parameter study, values of mean temperature and mean square temperature fluctuation are selected in order to examine effects of their variation on the mean turbulent Arrhenius reaction rate constant. The results of this study are presented in

Section 5 for comparison with the results obtained by utilizing the temperature-derived most-likely pdf in equation (29).

4. Joint Probability Density Functions for Temperature and Species

4.1 Most-likely Bivariate pdf

The most-likely pdf of Section 3 is easily extended to two or more variables (e.g., temperature and one species concentration; temperature and two species concentrations, etc.). The form of the most-likely bivariate pdf for temperature and one species concentration is:[2]

$$p(r_F, t) = q \cdot (\lambda_0 + \lambda_1 t + \lambda_2 r_F + \lambda_3 t r_F) \tag{33}$$

where q = *a priori* probability dependent upon the reaction rate

t = dimensionless temperature

r_F = dimensionless concentration of fuel, H_2

$\lambda_0, \lambda_1, \lambda_2, \lambda_3$ = constants

The constant coefficients $\lambda_0, \lambda_1, \lambda_2, \lambda_3$ are determined from the simultaneous solution of the following constraint equations for known values of $\overline{r_F}$, $\overline{t}$, $\overline{r_F'^2}$, $\overline{t'^2}$ and ρ:

$$\int_0^1 \int_0^1 p(r_F, t)\, dr_F\, dt = 1 \tag{34}$$

$$\int_0^1 \int_0^1 r_F \cdot p(r_F, t)\, dr_F\, dt = \overline{r_F} \tag{35}$$

$$\int_0^1 \int_0^1 t \cdot p(r_F, t)\, dr_F\, dt = \overline{t} \tag{36}$$

$$\int_0^1 \int_0^1 (r_F - \bar{r}_F)(t - \bar{t}) \cdot p(r_F, t)\, dr_F\, dt = \overline{r_F' t'} \quad (37)$$

Equation (34) follows from equation (2). Equations (35) and (36) are expressions for the dimensionless mean concentration of fuel species and dimensionless mean temperature, respectively. Equation (37) is the expression for the covariance of the dimensionless fuel species concentration r_F and the dimensionless temperature t.

For a given value of $\bar{t}$ and $\bar{r}_F$, the value of the covariance is obtained by utilizing equation (8). For the purposes of this study, an approximate value of the correlation is taken to be -0.9 from Reference (1), for an assumed adiabatic, turbulent diffusion flame. Hence,

$$\sigma_{r_F,t} = \overline{r_F' t'} = \rho_{r_F t} \sqrt{\overline{r_F'^2} \cdot \overline{t'^2}} \quad (38)$$

where $\rho_{r_F t} = -0.9$

In addition, in order to utilize equations (35), (36), (37), and (38), the following relationships from Reference (1) are employed:

$$\bar{r}_F = 1 - \bar{t} \quad (39)$$

$$\overline{r_F'^2} = \frac{2}{3} \overline{t'^2} \quad (40)$$

The "ϵ_{ω}" term appearing in equation (33) is an a priori probability dependent upon the reaction rate. In the present study, t and r_F are treated as passive scalars. This simplification is seen as an initial step in the utilization of the most-likely pdf. For this case, Reference (2) shows that the q-term is a constant. For purposes of calculation, this term is set equal to unity.

Equation (33) may be utilized in equation (19) to obtain the following expression for the mean turbulent reaction rate:

$$\overline{\dot{w}}_t = -A \int_0^1 \int_0^1 (K_1 t + K_2)^B \cdot \exp\left[-T_A/(K_1 t + K_2)\right] r_F c_F^\circ \cdot \left[\nu c_F^\circ (r_F - 1) + c_0^\circ\right] \cdot p(t, r_F)\, dt\, dr_F \tag{41}$$

where $p(t, r_F)$ = most-likely bivariate pdf.

The corresponding "laminar" term is calculated by use of $\bar{t}$ and $\bar{r}_F$ in equation (17). Refecence (1) shows that equation (17) may be rewritten as:

$$\dot{w}_\ell = -K(t)\, r_F\, c_F^\circ \left[\nu c_F^\circ (r_F - 1) + c_0^\circ\right] \tag{42}$$

The ratio of equation (41) to (42) is the reaction rate amplification ratio Z':

$$Z' = \frac{\overline{\dot{w}}_t}{\dot{w}_\ell} \tag{21}$$

For the purposes of a parameter study with the model given by equation (41), the following one-step, irreversible reaction is considered:

$$H_2 + \frac{1}{2} O_2 \longrightarrow H_2O \tag{43}$$

The results of this parameter study are presented in Section 5.

The computational procedure to determine the values of the reaction rate amplification ratio is described below.

Procedure

1. Choose values for A, B, T_A, Tmin, Tmax, $\bar{t}$ and $\overline{t'^2}$
2. Utilize Newton's Method to solve for the constant coefficients of equation (33).
3. Numerically integrate equation (41) to obtain $\bar{\dot{w}}_t$.
4. Insert $\bar{t}$ and $\bar{r}$ into equation (42) to obtain $\dot{w}_\ell$.
5. Calculate Z' with equation (21).

4.2 Modified Bivariate Gaussian pdf

This is an alternative two-dimensional pdf, as initially presented in Reference (1) and is given by equation (44):

$$f(t,r) = \frac{p(t,r)}{\int_0^1 \int_0^1 p(t,r)\,dt\,dr} \quad ; \quad \begin{array}{l} 0 \le t \le 1 \\ 0 \le r \le 1 \end{array} \tag{44}$$

In the above equation, p(t,r) is the bivariate Gaussian pdf given by:

$$p(t,r) = \frac{1}{2\pi\sigma_t\sigma_r\sqrt{1-\rho^2}} \cdot \left\{ \exp\left[-\frac{1}{2(1-\rho^2)} \left[\frac{(t-\mu_t)^2}{\sigma_t^2} - \frac{2\rho(t-\mu_t)(r-\mu_r)}{\sigma_t\sigma_r} + \frac{(r-\mu_r)^2}{\sigma_r^2} \right]\right]\right\}$$

$$\text{for} \quad \begin{array}{l} -\infty < t < \infty \\ -\infty < r < \infty \end{array}$$

Equation (44) is utilized in equation (19) to obtain the following expression for the mean turbulent reaction rate:

$$\bar{\dot{w}}_t = -A \int_0^1 \int_0^1 (K_1 t + K_2)^B \cdot \exp\left[-T_A/(K_1 t + K_2)\right] \cdot r_F c_F^\circ \left[\nu c_F^\circ (r_F - 1) + c_o^\circ\right] \cdot f(t, r_F)\, dt\, dr_F \quad (45)$$

where $f(t, r_F)$ = modified bivariate Gaussian pdf.

Discussion of the modified bivariate Gaussian pdf and the procedure for utilizing equation (45) are given in Reference (1).

The ratio of equation (45) to (42) is the reaction rate amplification ratio, Z':

$$Z' = \frac{\bar{\dot{w}}_t}{\dot{w}_\ell} \quad (21)$$

The results of a parameter study with this model are presented in Reference (1). This parameter study considers the one-step, irreversible reaction given by equation (43). The results of the parameter study of Reference (1) are compared to those obtained by means of the most-likely bivariate pdf in Section 5.

5. Results

Throughout the discussion in this section, the use of the terms "temperature" and "concentration" denote mean dimensionless temperature and mean dimensionless species concentration, respectively. The use of "r" in all figures denotes r_{H_2}.

5.1 The Effects of Temperature Fluctuations on the Arrhenius Reaction Rate Constant

The effects of temperature fluctuations on the Arrhenius reaction rate constant are presented in this first subsection. The calculations are performed with the temperature-derived most-likely pdf. The results of these calculations are compared with those obtained by use of the beta pdf taken from Reference (1).

5.1.1 Computational Aspects

All numerical integrations are performed using Simpson's Rule. Newton's Method is used to solve for the unknown coefficients in equation (23). Details concerning this technique and the associated proof of convergence and error analyses will appear in the next progress report.

5.1.2 Discussion of Results

Table 1. shows the cases considered. The data presented are obtained from Reference (5) and are considered to be typical. All the following results are stated with regard to both the temperature-derived most-likely and beta pdf's. Proposed explanations for the phenomena involved are given in Reference (1).

Table 1. Case Data

Case No.	B	T_A (^oK)	T_{max} (^oK)
1	0	10116.	2500.
2	0	5000.	2500.
3	1	10116.	2500.
4	0	10116.	3000.

Note: $A = 8.4 \times 10^{13}$, $T_{min} = 500^oK$, for all cases.

Variation with mean temperature and temperature fluctuation

Figures 3. through 7. show the variation of the reaction rate constant amplification ratio with mean temperature and mean square temperature fluctuation. The following are observed:

1) The reaction rate constant amplification ratio increases with increasing values of mean square temperature fluctuation, at constant values of mean temperature for both pdf's. Refer to Figures 3. through 7.

2) The reaction rate constant amplification ratio decreases with increasing values of mean temperature fluctuation for both pdf's. Refer to Figures 3. through 7.

3) The same values of Z are obtained with the use of both pdf's for values of $\bar{t}$ = 0.5, 0.6. Refer to Figures 5. and 6.

4) Nearly the same values of Z are obtained with the use of both pdf's for values of $\bar{t}$ equal to 0.2 through 0.7 and, for $\bar{t}$ = 0.8 and $\overline{t'^2} \leq 0.04$.

Variation with activation temperature

Figure 8. shows the variation of the reaction rate constant amplification ratio with the activation temperature. As may be seen, a decrease in the activation temperature results in a similar decrease in Z for the two pdf's.

Variation with temperature exponent, B.

Figure 9. shows the variation of the reaction rate constant amplification ratio with the temperature exponent, B. It is observed that an increase in the temperature exponent results in similar increases in A, for both pdf's.

Variation with maximum temperature

Figures 10. and 11. show the variation of the reaction rate constant amplification ratio with the maximum temperature. It is seen that in both cases the value of Z is relatively insensitive to changes in Tmax.

From these results, it is concluded that quite similar results are obtained by the use of the beta and most-likely pdf's. Since the former has been experimentally verified in many non-reacting, turbulent flows, this similarity in behavior lends support to the physical correctness of the most-likely pdf.

5.2 Effects of Temperature and Species Fluctuations on the Reaction Rate

The effects of temperature and species concentrations fluctuations on the mean turbulent reaction rate are presented in this subsection. The calculations are performed with the most-likely bivariate pdf.(2) The results of these calculations are compared with those obtained by means of the modified bivariate Gaussian pdf taken from Reference (1).

5.2.1 Computational Aspects

During the course of this study, a method was developed to transform the double integrals of equations (34) through (37) to single integrals. This rendered the evaluation of the associated unknown constants practical by means similar to those mentioned in Section 5.1.1. Details of this transform method and the associated numerical techniques will appear in a future status report.

5.2.2 Discussion of Results

Table 2. shows the cases considered. The initial values of concentrations are taken from Reference (5). All other data are also taken from Reference (5) and are considered to be typical. All the following results are stated with regard to both the most-likely bivariate and modified bivariate Gaussian pdf's. Proposed explanations for the pheonomena involved are given in Reference (1).

Case No.	B	T_A (^oK)	T_{max} (^oK)	P	$\overline{r'^2_{H_2}}$ vs $\overline{t'^2}$
1	0	10116.	2500.	-0.9	$\overline{r'^2_{H_2}} = 2/3\ \overline{t'^2}$
4	0	10116.	3000.	-0.9	"
5	0	10116.	2500.	-0.8	"
6	0	10116.	2500.	-0.9	$\overline{r'^2_{H_2}} = 1/2\ \overline{t'^2}$

Note: $A = 8.4 \times 10^{13}$, Tmin = 500^oK, $C^o_{H_2} = 2.405 \times 10^{-5}$ gmol/cm^3, $C^o_{O_2} = 1.5 \times 10^{-6}$ gmol/cm^3, $\bar{r}_{H_2} = 1-\bar{t}$, for all cases.

<u>Variation with fluctuations and mean values of temperature and species</u>

Figures 12. through 17. show the variation of the reaction rate amplification ratio with temperature and species fluctuations,

at various constant values of mean temperature and mean concentration. These results consider combined effects of temperature and species fluctuations. The following are observed:

1) The reaction rate amplification ratio increases with increasing values of fluctuations for values of $\bar{t}$ from 0.2 through 0.5. Refer to Figures 12. through 15.

2) The reaction rate amplification ratio reaches a relative maximum and then decreases with increasing fluctuations at $\bar{t} = 0.6$. Refer to Figure 16.

3) The reaction rate amplification ratio decreases with increasing fluctuations and is less than unity at $\bar{t} = 0.7$. Refer to Figure 17. The implication of $Z' < 1$ is that species fluctuations are resulting in an "unmixedness" effect which is reducing the turbulent reaction rate to values less than the "laminar"-calculated values.

4) The reaction rate amplification ratio decreases with increasing values of $\bar{t}$ (and correspondingly decreasing values of $\bar{r}$) at constant values of fluctuations. Refer to Figures 12. through 17. This implies that in this turbulent flame, the principal turbulent amplification is occurring in the region of flame initiation.

5) The use of the most-likely bivariate pdf yields values of Z' greater than, equal to and less than values obtained with the use of the modified bivariate Gaussian pdf, for values of $\bar{t} = 0.2$, 0.3 and 0.4. Refer to Figures 12., 13., and 14.

6) The use of the most-likely bivariate pdf always yields values of Z' greater than the values obtained with the use of the modified bivariate Gaussian pdf for values of $\bar{t}$ = 0.5, 0.6, 0.7. Refer to Figures 15., 16. and 17. The results obtained in the previous section lend greater credence to the values obtained using the most-likely bivariate pdf.

Figure 18 reveals that both joint pdf's are sensitive to the value selected for T_{max}, which was not the case for the temperature-only pdf's.

Variation with the correlation coefficient

Figure 19. shows the variation of the reaction rate amplification ratio with the correlation coefficient. It is observed that the value of Z' exhibits a relatively small decrease with an 11% increase in the value of ρ.

Variation with $\overline{r'^2_{H_2}}$ vs $\overline{t'^2}$

Figure 20. shows the variation in the reaction rate amplification ratio with an approximate change of 30% (2/3 to 1/2), in the relationship between $r'^2_{H_2}$ and $\overline{t'^2}$. The following are observed:

1) The value of Z' is generally lowered by this.
2) The decrease in Z' is substantial with the use of the most-likely bivariate pdf. This suggests that the most-likely pdf will serve as a more sensitive indicator of the correctness of a given turbulence-reaction model, when compared with the modified Gaussian.

5.3.1 Discussion of Results

Variation with fluctuations and mean temperature

Figures 21. through 26. show comparisons of the variation of the reaction rate amplification ratio for the two-variable and one-variable models with values of the fluctuations and mean temperature.

The following are observed:

1) The reaction rate amplification ratio increases with increasing temperature fluctuations at constant values of $\bar{t}$, for $\bar{t}$ = 0.2 through 0.5. This trend is realized for both the one-variable and two-variable models. Refer to Figures 21. through 24.

2) The value of Z' decreases with increasing $\bar{t}$ at constant values of $\overline{t'^2}$ for both the one-variable and two-variable models. Refer to Figures 21, through 26.

3) The value of Z' increases with increasing temperature fluctuations at $\bar{t}$ = 0.6, with the use of the one-variable model. Also at this value of $\bar{t}$, Z' increases, reaches a relative maximum, then decreases with increasing temperature fluctuations, with the use of the two-variable model. Refer to Figure 25.

4) The value of Z' increases with increasing temperature fluctuations at $\bar{t}$ = 0.7, with the use of the one-variable model. For all values of $\overline{t'^2}$, this model yields values of $Z > 1$. At this same value of $\bar{t}$, Z' decreases with increasing temperature fluctuations and is always less than unity, with the use of the two-variable model. Refer to Figure 26.

These results clearly indicate the necessity for multi-dimensional pdf models since, in temperature-only models, the species "unmixedness" reduction in the reaction rates ($Z < 1$) is totally absent.

6. Conclusions and Direction of Future Work

6.1 Conclusions

6.1.1 Effect of Temperature Fluctuations on the Arrhenius Reaction Rate Constant

The effects of temperature fluctuations on the Arrhenius reaction rate constant are assessed by treating the temperature as a continuous random variable and utilizing two pdf's for temperature. The pdf's are the temperature-derived most-likely and the beta. The ratio of the mean turbulent Arrhenius reaction rate constant to the corresponding laminar term is defined as the amplification ratio, Z. The results obtained by means of both pdf's exhibit the following trends:

1. Z is always greater than unity.
2. Z increases as $\overline{t'^2}$ increases, at constant $\bar{t}$
3. Z decreases as $\bar{t}$ increases, at constant $\overline{t'^2}$
4. For wide ranges of $\bar{t}$ and $\overline{t'^2}$, the use of both pdf's yields nearly identical numerical results.
5. Z is relatively insensitive to moderate changes in T_A and B.
6. Z is insensitive to moderate changes in T_{max}.

6.1.2 Effects of Temperature and Species Fluctuations on the Reaction Rate

The effects of temperature and species fluctuations on the reaction rate are assessed by treating both the temperature and species concentration as continuous random variables and utilizing joint pdf's relating them. The pdf's are the most-likely bivariate and modified bivariate Gaussian.

A reaction rate amplification ratio Z' is defined at the ratio of a mean turbulent reaction rate to the corresponding laminar term. Also defined is a reaction rate amplification ratio with a mean turbulent reaction rate composed of a mean turbulent Arrhenius reaction rate constant and laminar values of concentration. This amplification ratio only considers the effect of temperature fluctuations on the reaction rate. It is possible to compare the combined effects of temperature and species fluctuations to those of only temperature fluctuations by comparison of the two-variable (temperature and species) and the one-variable (temperature) models. These one-variable models utilize the temperature derived most-likely and beta pdf's. The results of the two-variable models exhibit the following trends:

1. Z' of the combined case may be greater than, equal to or less than that of the temperature-only case.
2. Z' of the combined case increases with increasing temperature and species concentration fluctuations, at low values of mean temperature and correspondingly high values of mean species concentration. At high values of temperature and correspondingly low values of concentration, Z' decreases with increasing fluctuations.
3. Z' of the combined case is sensitive to changes in T_{max}.
4. Z' of the combined case is nearly insensitive to small changes in ρ.

5. The values of Z' obtained with the use of the most-likely bivariate pdf are moderately sensitive to changes in the relationship between temperature and species fluctuations. The values of Z' obtained with the use of the modified bivariate Gaussian pdf is insensitive to moderate changes in this same relationship.

6.2 Direction of Future Work

1. Continue development of a temperature-two species fluctuations model (previously identified as model II, Reference 1c).
2. Evaluate the "q" term in equation (33) to allow the treatment of reactive scalars.
3. Utilize the three-variable analog of equation (33) in order to eliminate the assumption on which equation (41) is based (previously identified as model III, Reference 1c).

7. Development of a Criterion for the use of the Ramp PDF

7.1 Introduction

A criterion for selecting between the beta (or one-dimensional most-likely) and ramp pdf's is under investigation. The flatness factor and skewness are studied for potential use as criteria. The ramp pdf generates values of flatness factor between 2.0 and 2.5. The beta pdf also generates these values of the flatness factor since it is a continuous distribution (its range of flatness is 1.66 and 8.64.) However, when the flatness factor is between 2.0 and 2.5, the skewness for each of the pdf's is distinct. This leads one to choose skewness as a secondary criterion with flatness factor being primary.

A comparison of the beta and most-likely pdf's is made with the conclusion that they do not yield equivalent values for the higher order moments.

7.2 Moments of a pdf

Every probability density function (pdf) has an infinite number of moments associated with it. The most commonly used moment is the first, called the mean, μ. The mean is defined as:

$$\mu = \int_{-\infty}^{\infty} t \cdot p(t)\,dt \tag{46}$$

Alternatively, $\mu = \bar{t}$ may be used. This moment is also called the expected value, E(t).

The second moment is the variance, V. The square root of the variance is the standard deviation, σ, and is given by:

$$\sigma^2 = \int_{-\infty}^{\infty} (t-\mu)^2 \cdot p(t)\,dt \tag{47}$$

If the polynomial is expanded and multiplied through by p(t), one obtains

$$\sigma^2 = \int_{-\infty}^{\infty} t^2 \cdot p(t)\,dt - 2\mu\int_{-\infty}^{\infty} t \cdot p(t)\,dt + \mu^2\int_{-\infty}^{\infty} p(t)\,dt \tag{48}$$

The only factor that is not known in Equation (48) is

$$E(t^2) = \int_{-\infty}^{\infty} t^2 \cdot p(t)\,dt \tag{49}$$

Similarly, higher order moments will also contain a term of the same form, or

$$E(t^k) = \int_{-\infty}^{\infty} t^k \cdot p(t)\,dt \tag{50}$$

where k is the moment desired.

In order to calculate any moment, it is sufficient to calculate $E(t^k)$ and then multiply by the appropriate constants to obtain the moment desired.

Moments higher than 2 are given by the following general equation:

$$M_N = \frac{1}{\sigma^N} \cdot \int_{-\infty}^{\infty} (t-\mu)^N \cdot p(t)\,dt \tag{51}$$

Note that expansion of the $(t-\mu)^N$ term will yield the term $t^N\, p(t)\, dt$.

The third moment is called the skewness, and the fourth is called the flatness factor.

7.3 Moments of the Beta pdf

The beta pdf, proposed by Rhodes (6) to describe turbulent flow properties, is given by:

$$p(t) = \frac{t^{a-1}(1-t)^{b-1}}{\int_0^1 t^{a-1}(1-t)^{b-1}\,dt} \tag{52}$$

where

$$a = \bar{t}\left[\frac{\bar{t}(1-\bar{t})}{\overline{t'^2}} - 1\right] \tag{53}$$

and

$$b = (1-\bar{t})\left[\frac{\bar{t}(1-\bar{t})}{\overline{t'^2}} - 1\right] \tag{54}$$

The denominator of Equation (52) can be expressed using the Gamma function:

$$\int_0^1 t^{a-1}(1-t)^{b-1}\,dt = \frac{\Gamma(a)\cdot\Gamma(b)}{\Gamma(a+b)} \tag{55}$$

The moments of the Beta pdf are

$$M_N = \frac{1}{\sigma^N}\int_0^1 (t-\mu)^N\cdot p(t)\,dt \quad (N \geq 2) \tag{56}$$

where μ is the mean. If the polynomial in Equation (56) is expanded, there is always a $\int t^M p(t)\, dt$ term to be evaluated. It can be evaluated using a form of Equation (55):

$$\int_0^1 t^{x-1}(1-t)^{y-1}\,dt = \frac{\Gamma(x)\cdot\Gamma(y)}{\Gamma(x+y)} \tag{57}$$

$$E(t^K) = \frac{\Gamma(a+b)}{\Gamma(a)\cdot\Gamma(b)}\cdot\int_0^1 t^K t^{a-1}(1-t)^{b-1}\,dt$$

$$= \frac{\Gamma(a+b)}{\Gamma(a)\cdot\Gamma(b)}\cdot\int_0^1 t^{K+a-1}(1-t)^{b-1}\,dt \tag{58}$$

If one lets x in Equation (57) equal (k+a) and y=b, then

$$E(t^K) = \frac{\Gamma(a+b)}{\Gamma(a)\cdot\Gamma(b)}\cdot\frac{\Gamma(a+K)\cdot\Gamma(b)}{\Gamma(a+b+K)}$$

$$\int_0^1 t^K\cdot p(t)\,dt = E(x^K) = \frac{\Gamma(a+b)\cdot\Gamma(K+a)}{\Gamma(a)\cdot\Gamma(K+a+b)} \tag{59}$$

Equation (59) has been used to evaluate the moments. The skewness and flatness factor distributions as functions of $\bar{t}$ and $\overline{t'^2}$ are shown in Figures 27 - 30. The distribution is symmetric about $\bar{t}=0.5$, therefore only one graph is needed for both $\bar{t}=0.4$ and $\bar{t}=0.6$ since they have the same values. The only difference is in the skewness - for $\bar{t}=0.4$, the skewness is positive, for $\bar{t}=0.6$, the skewness has the same magnitude but is opposite in sign. The same holds true for $\bar{t}=0.1,0.9$; $\bar{t}=0.2,0.8$; $\bar{t}=0.3,0.7$, etc.

7.4 Moments of the Pope Pdf

The most-likely pdf proposed by Pope[2,7] has the form:

$$p(t) = e^{\lambda_0 + \lambda_1 t + \lambda_2 t^2} \tag{60}$$

where λ_o, λ_1, λ_2 are three constants which are functions of $\bar{t}$ and $\overline{t'^2}$. Since there are three unknowns, three equations are required to determine the three constants. However, only two algebraic equations can be developed (Appendix B):

$$e^{\lambda_0 + \lambda_1 + \lambda_2} - \lambda_1 t - 2\lambda_2(\overline{t'^2} - \bar{t}^2) = 1 \tag{61}$$

$$e^{\lambda_0} = \frac{2\lambda_2 \bar{t} + \lambda_1}{e^{\lambda_1 + \lambda_2} - 1} \tag{62}$$

The required third equation is an integral equation defining one of the properties of a pdf, or its first two moments, namely

$$\int_0^1 p(t)\,dt = 1 \tag{63}$$

$$\int_0^1 t \cdot p(t)\,dt = \bar{t} \tag{64}$$

$$\int_0^1 (t-\mu)^2 \cdot p(t)\,dt = \overline{t'^2} \tag{65}$$

Any one of these three equations can be used as the third equation.

Once the three λ's are known, the higher order moments can be found using the following equation:

$$M_N = \frac{1}{\sigma_N} \int_0^1 (t-\bar{t})^N \cdot e^{\lambda_0 + \lambda_1 t + \lambda_2 t^2}\,dt \tag{66}$$

Graphs of the skewness and flatness factor as a function of $\bar{t}$ and $\overline{t'^2}$ are presented in Figures 27 - 30. As with the beta pdf, the values of the flatness factor are symmetric about $\bar{t}=0.5$. That is, the same values of the flatness factor are obtained for $\bar{t}=0.4$ and $\bar{t}=0.6$. The same is true for the skewness, except that the signs are reversed (negative values when $\bar{t}\geq 0.5$). One interesting phenomenon encountered was that there seemed to be no solution obtainable for some $\overline{t'^2}$ when $\bar{t}=0.1$ or 0.9. Some data points were obtained, but not enough to permit a comparison with other pdf's.

7.5 Comparison between the Beta vs. Pope Pdf's

The behavior of the beta and Pope pdf's is very similar near $\bar{t}=0.5$. As can be seen from Figure 30, both curves follow the same trend and approach each other at high $\overline{t'^2}$. At $\bar{t}=0.4, 0.6$, the flatness factor curves are fairly similar and approach each other at high values of the fluctuations. The skewness curves are not as similar as the flatness curves.

The differences between the pdf's becomes more pronounced at $\bar{t}=0.3,0.7$. The skewness curves are essentially the same except they are a little further apart. The flatness factor curves are distinct now as the Pope pdf has a maximum while the beta does not. At the maximum, the flatness factor for the Pope pdf is approximately 13% higher than for the beta pdf.

At $\bar{t}=0.2,0.8$, there is a large difference in the flatness factor curves. Both curves have a maximum, but the Pope pdf has a much more pronounced peak. The skewness curves have basically the same shape as before, but again are further apart.

The two skewness curves always cross each other, with the point of intersection moving to the right with increasing $\bar{t}$. After the intersection, the Pope pdf yields higher values than the beta pdf.

The conclusion that can be drawn from these curves is that the beta and Pope most-likely pdf's yield values for the higher-order moments which can differ substantially. Both encompass the same range of values, but the differences are such that, on this basis, they are not interchangeable.

7.6 Moments of the Ramp pdf

The ramp pdf was developed by Antonia and Atkinson[8] after observing ramp-like temperature fluctuations under a variety of conditions. The pdf is composed of two parts - a ramplike structure with high -frequency Gaussian fluctuations superimposed. The general equation for the ramp pdf is:

$$p(r^*) = \frac{c^{\beta-1}}{\alpha'(1-r^*)} \cdot \Gamma\left[1-\frac{1}{\beta}, c\left(\frac{1}{\alpha'} \ln(1-r^*)^{-1}\right)^{\beta}\right] \tag{67}$$

where the incomplete Gamma function is defined as

$$\Gamma(a,x) = \int_x^{\infty} t^{a-1} e^{-t}\, dt \tag{68}$$

There are 4 constants in equation (22) which are adjustable: α',β,c, and σ* (σ* is an implicit normalizing factor.) Antonia et.al. have shown that if α'=1.8,β=1.25, c=1.0, and σ*=0.25, good correlation with experimental results is obtained. (For a fuller discussion of the ramp pdf and its properties, see reference (1).) The equation to evaluate the expected values (which leads to the moments) for the ramp pdf is [1]:

$$E(t^{*N}) = \int_0^1 \frac{c^{\beta-1}}{\alpha'(1-r^*)}\left[\int_x^{20} (r^*)^{a-1} \cdot e^{-r^*} dr^*\right]\left[r^{*N} + \left(2^{N-2} + (N-2)\right) r^{N-2}\sigma^{*2} + 3r^{*N-4}\sigma^{*4}\right] dr^* \tag{69}$$

The effect of changes in the four adjustable constants on the skewness and flatness factor is shown in Figures 31 - 34. It can be seen that the skewness and flatness factor are very sensitive to changes in σ*. Varying σ* from 0.1 to 0.5 will yield values of F between 1.0 and 3.7. This sensitivity requires that σ* be selected in accordance with the best-available experimental data. Antonia[8] indicates that a value of σ*=0.25 yields very good agreement with his experimental data.

With σ^* held constant at $\sigma^*=0.25$ and the other constants varied, the flatness factor ranges approximately between 2.0 and 2.5. This is in agreement with Fiedler[9] who predicted that a value of 2 was characteristic of the sawtooth-like ramp pdf. The range of the skewness was -1.57 to -1.25.

The skewness and flatness factor distributions for the beta pdf are shows in Figures 27 - 30. The flatness factor ranges from 1.66 to 8.64. Since the beta pdf is continuous, every intermediate value can be obtained by the proper selection of $\bar{t}$ and $\overline{t'^2}$. This means that the beta pdf will likewise generate the values 2.0-2.5 for the flatness factor. However, the beta pdf generates values of skewness between -2.66 and +2.66. When the flatness factor lies between 2.0 and 2.5, the skewness varies between -0.82 and +0.82. Recalling that the ramp pdf has skewness values between -1.57 and -1.25 for the same range of flatness factors, implies that the skewness can be used as the secondary criterion for distinguishing between the two pdf's.

The procedure is as follows: if the flatness factor lies <u>outside</u> the range 2.0 - 2.5, then always choose the beta pdf since the ramp pdf does not produce these values. When the flatness is between 2.0 and 2.5, both pdf's can take on these values; hence, the skewness must be consulted. If the skewness is greater than -0.82, choose the beta pdf; if less than -1.25, select the ramp pdf.

A simpler, though less general, secondary criteron is to determine if the skewness is positive or negative. If it is positive, choose the beta pdf since the ramp pdf can only produce negative values for the skewness. If it is negative, the method indicated in the last paragraph must be used.

. The skewness alone cannot be used as a criterion because the values generated by the two pdf's are not distinct, but overlap. The full range of the skewness values for the ramp pdf is -1.57 to -1.25; and the range of the Beta pdf is -2.66 to +2.66.

In order to determine values for the skewness and flatness factor in a turbulent, reacting flow, a transport equation is being developed that will enable the determination of these quantities.

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List of Symbols

A	pre-exponential constant
B	temperature exponent
C	instantaneous concentration
C^o	initial concentration
E(x)	expected (mean) value of x
F	denotes a fuel species
f(x,y)	joint probability density function of (x,y)
g(x,y)	function of the two-dimensional continuous random variable (x,y)
$\overline{g(x,y)}$	mean value of g(x,y)
h(x)	function of the continuous random variable, x
K	Arrhenius reaction rate constant
K_1, K_2	constants dependent upon Tmin and Tmax
K_ℓ	laminar Arrhenius reaction rate constant
$\overline{K_t}$	mean turbulent Arrhenius reaction rate constant
m	constant, defined in equation (30)
max	denotes maximum value
min	denotes minimum value
n	order of reaction constant
O	denotes oxidizer species
P	denotes a product species
p(x)	probability density function of x
p(x,y)	joint probability density function of (x,y)
r	dimensionless concentration and constant defined by equation (30)
$\bar{r}$	mean dimensionless concentration
$\overline{r'^2}$	mean square fluctuation of dimensionless concentration
t	dimensionless temperature
$\bar{t}$	mean dimensionless temperature
$\overline{t'^2}$	mean square fluctuation of dimensionless temperature
T	temperature

T_A	activation temperature
$V(x)$	variance of x
V'	value of integral defined by equation (44)
$\dot{w}$	reaction rate
$\dot{w}_\ell$	laminar reaction rate
$\overline{\dot{w}_t}$	mean turbulent reaction rate
Z	reaction rate constant amplification ratio
Z'	reaction rate amplification ratio
Γ	gamma function
μ_x	mean of a continuous random variable, x
μ_k'	Kth moment of a random variable
σ^2	variance of a continuous random variable
ρ	correlation coefficient

APPENDIX: Moments of the Pope Most-Likely PDF

$$\int_0^1 p(t)\,dt = 1 \tag{1}$$

$$\int_0^1 t\cdot p(t)\,dt = \bar{t} \tag{2}$$

$$\int_0^1 (t-\bar{t})^2\cdot p(t)\,dt = \overline{t'^2} \tag{3}$$

where

$$p(t) = \exp\left(\lambda_0 + \lambda_1 t + \lambda_2 t^2\right) \tag{4}$$

Integrate Eq. (1) by parts

$$u = p(t) \quad , v = t$$

$$du = (\lambda_1 + 2\lambda_2 t)\cdot p(t)\,dt \quad , dv = dt$$

$$\therefore \int_0^1 p(t)\,dt = 1 = t\cdot p(t)\Big|_0^1 - \int_0^1 t\,(\lambda_1 + 2\lambda_2 t)\cdot p(t)\,dt$$

$$e^{(\lambda_0+\lambda_1+\lambda_2)} - \int_0^1 \lambda_1 t\cdot p(t)\,dt - \int_0^1 2\lambda_2 t^2\cdot p(t)\,dt = 1$$

$$e^{(\lambda_0+\lambda_1+\lambda_2)} - \lambda_1\bar{t} - 2\lambda_2\int_0^1 t^2\cdot p(t)\,dt = 1 \tag{5}$$

Use Eq. (3) to eliminate the $\int t^2 \cdot p(t)\,dt$ term.

$$\int_0^1 (t^2 - 2t\bar{t} + \bar{t}^2) \cdot p(t)\,dt = \overline{t'^2}$$

$$\int_0^1 t^2 \cdot p(t)\,dt - 2\bar{t}\int_0^1 t\,p(t)\,dt + \bar{t}^2\int_0^1 p(t)\,dt = \overline{t'^2}$$

$$\int_0^1 t^2 \cdot p(t)\,dt - 2\bar{t}\cdot\bar{t} + (\bar{t})^2(1) = \overline{t'^2}$$

$$\int_0^1 t^2 \cdot p(t)\,dt = \overline{t'^2} + \bar{t}^2 \tag{6}$$

Substitute Eq. (6) into Eq. (5) to obtain:

$$e^{\lambda_0 + \lambda_1 + \lambda_2} - \lambda_1\bar{t} - 2\lambda_2\left[\overline{t'^2} + \bar{t}^2\right] = 1 \tag{7}$$

Equation (7) is one equation that contains only λ_o, λ_1, λ_2 plus constants.

$$e^{\lambda_0} = \frac{1 + \lambda_1\bar{t} + 2\lambda_2\left(\overline{t'^2} + \bar{t}^2\right)}{e^{\lambda_1 + \lambda_2}} \tag{7a}$$

To obtain another equation, start with Eq. (2):

$$\int_0^1 t \cdot e^{\lambda_0 + \lambda_1 t + \lambda_2 t^2}\,dt = \bar{t}$$

Since $\int e^x dx = e^x$, we would like the derivative of the exponent to precede the exponential term. This is done by multiplying and adding appropriate terms until $(\lambda_1 + 2\lambda_2 t)$ is obtained.

$$\int_0^1 2\lambda_2 t \cdot e^{\lambda_0 + \lambda_1 t + \lambda_2 t^2} dt = 2\lambda_2 \bar{t}$$

$$\int_0^1 2\lambda_2 t \cdot e^{\lambda_0 + \lambda_1 t + \lambda_2 t^2} dt + \int_0^1 \lambda_1 \cdot e^{\lambda_0 + \lambda_1 t + \lambda_2 t^2} dt =$$

$$2\lambda_2 \bar{t} + \int_0^1 \lambda_1 e^{\lambda_0 + \lambda_1 t + \lambda_2 t^2} dt$$

$$\int_0^1 (2\lambda_2 t + \lambda_1) e^{\lambda_0 + \lambda_1 t + \lambda_2 t^2} dt = 2\lambda_2 \bar{t} + \lambda_1$$

$$e^{\lambda_0 + \lambda_1 t + \lambda_2 t^2} \Big|_0^1 = 2\lambda_2 \bar{t} + \lambda_1$$

$$e^{\lambda_0 + \lambda_1 + \lambda_2} - e^{\lambda_0} = 2\lambda_2 \bar{t} + \lambda_1 \qquad (8')$$

$$e^{\lambda_0} = \frac{2\lambda_2 \bar{t} + \lambda_1}{e^{\lambda_1 + \lambda_2} - 1} \qquad (8)$$

Eqs. (7) and (8) are two equations in three unknowns. The third equation may be any one of the Eqs. (1), (2), or (3).

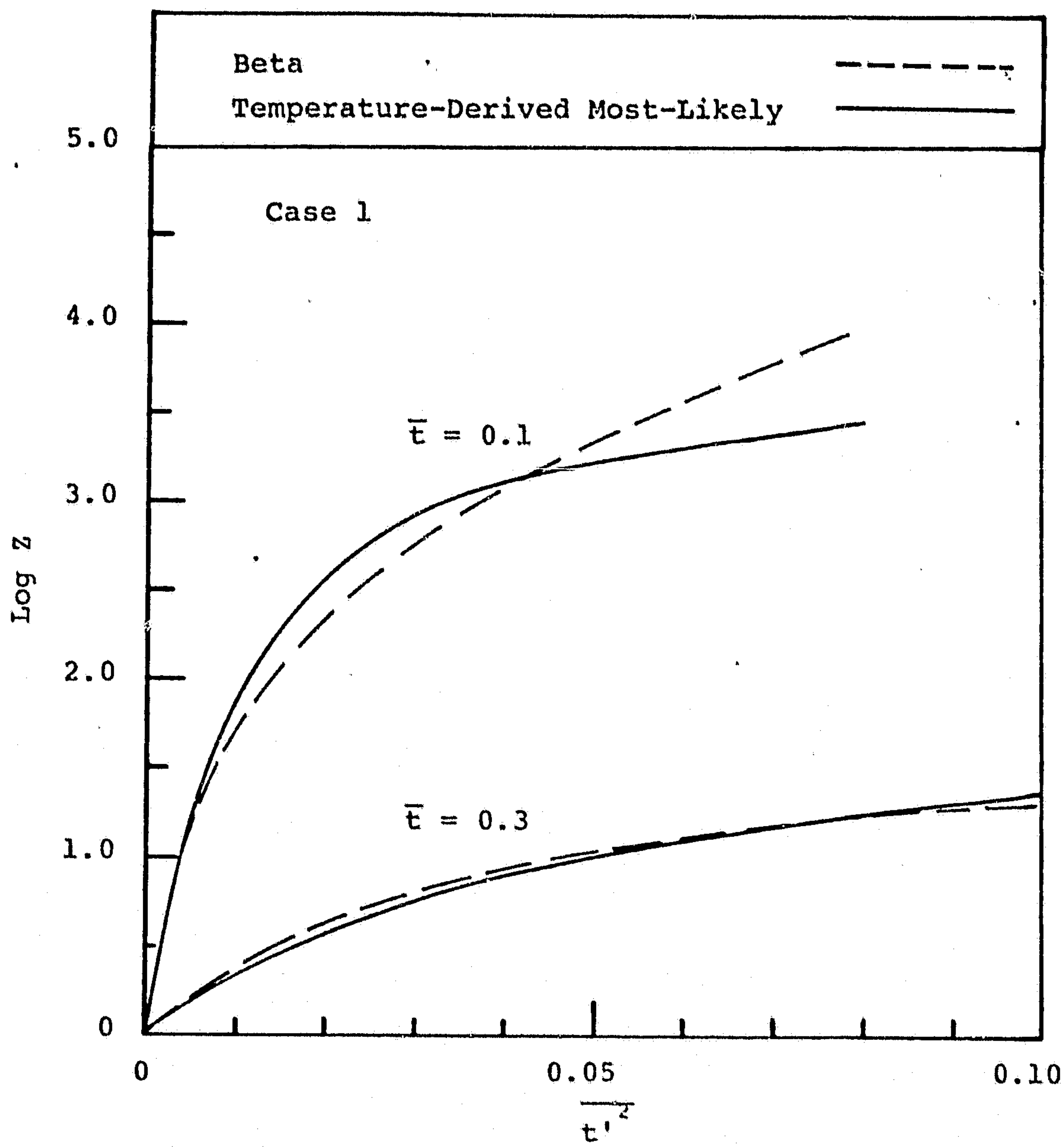


Figure 3. Variation of the reaction rate constant amplification ratio with the temperature fluctuation

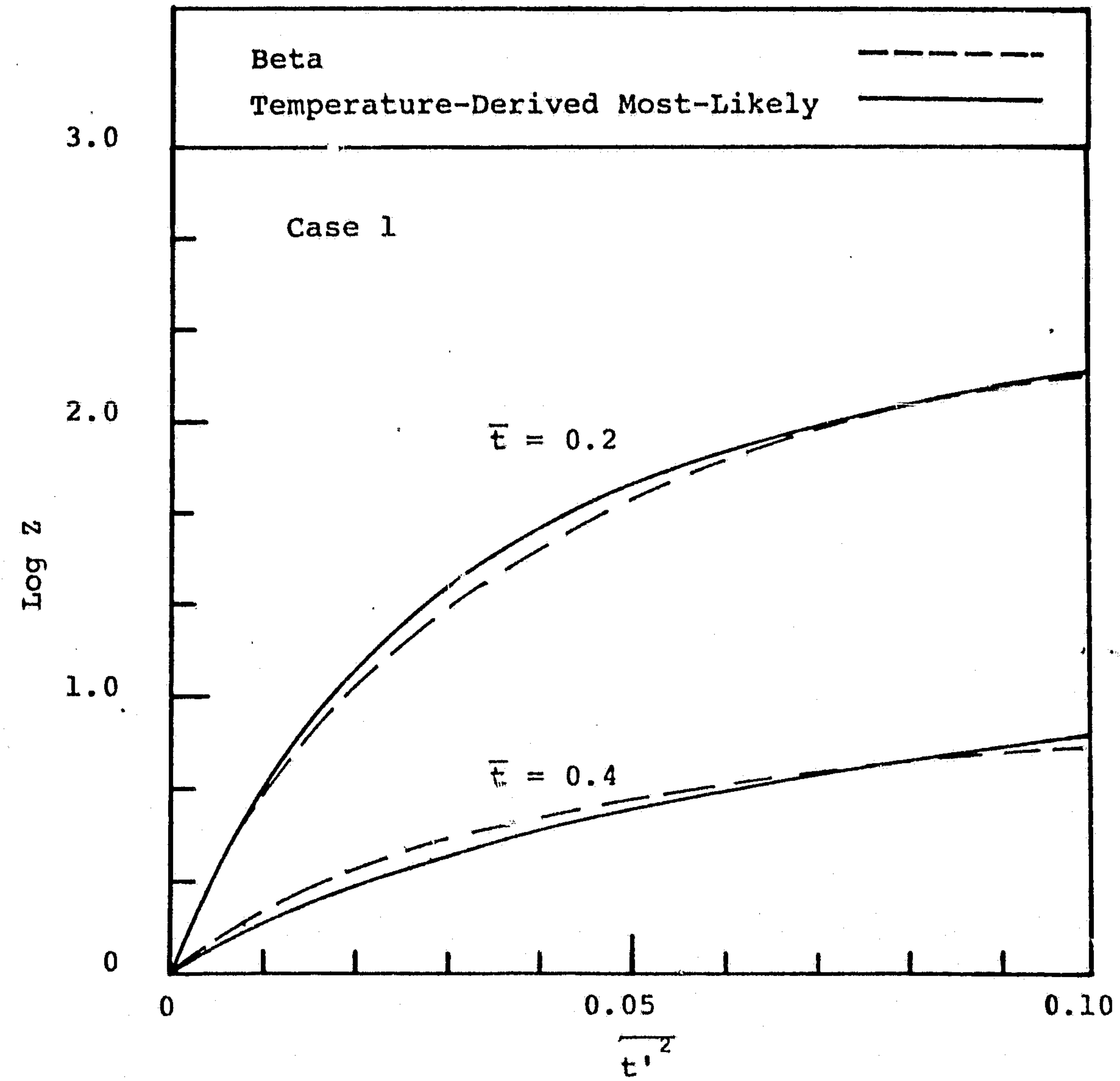


Figure 4. Variation of the reaction rate constant amplification ratio with the temperature fluctuation

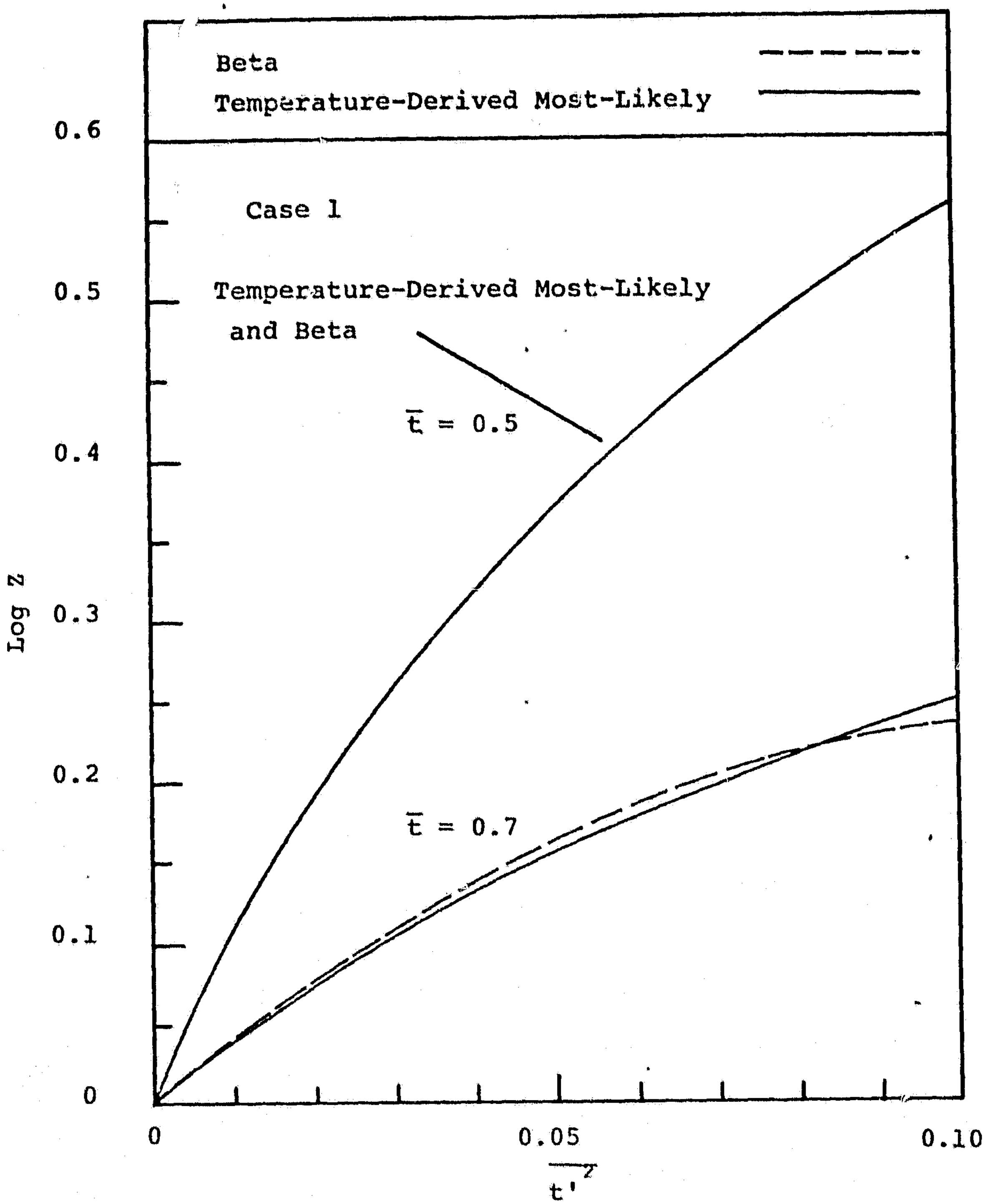


Figure 5. Variation of the reaction rate constant amplification ratio with the temperature fluctuation

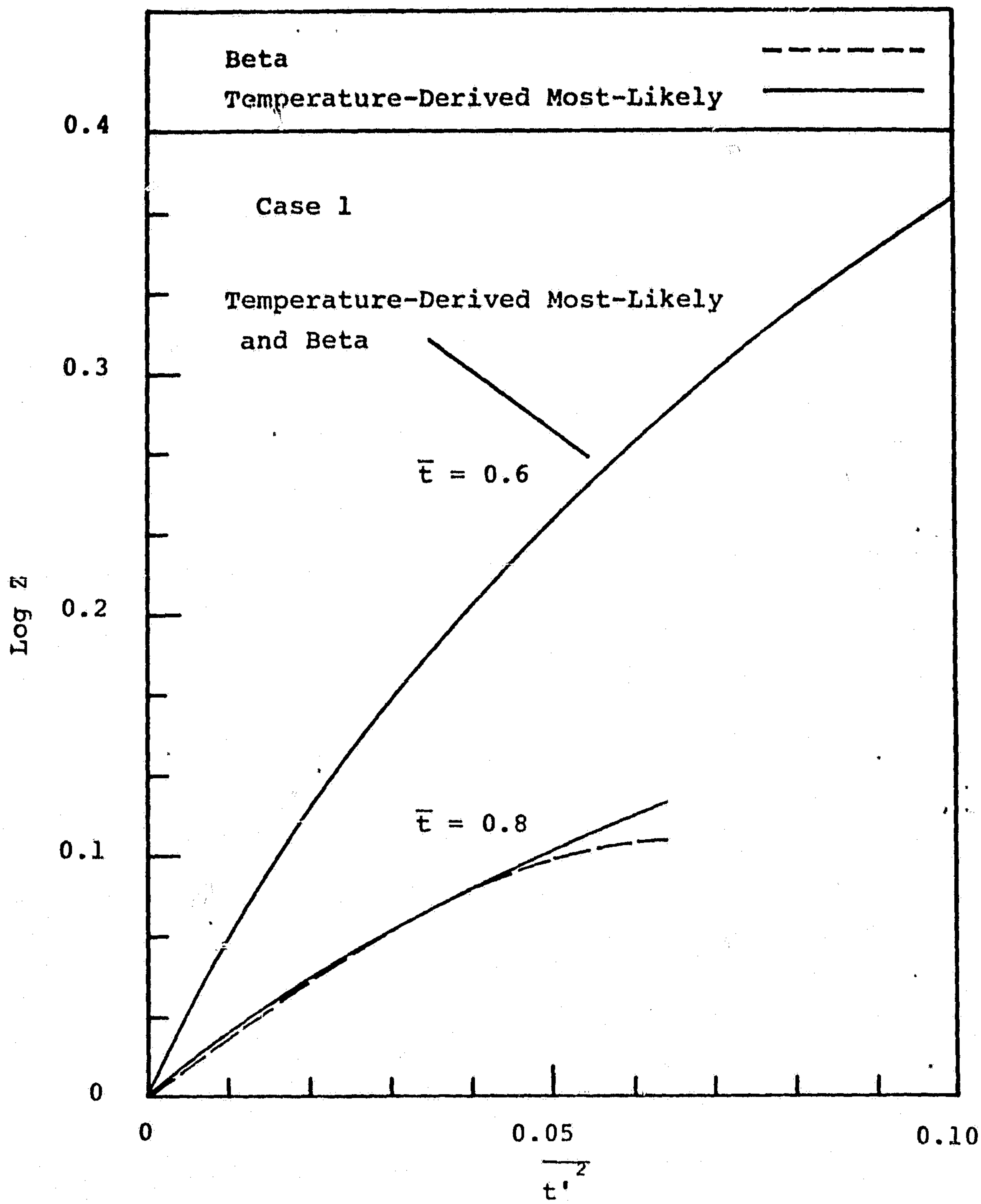


Figure 6. Variation of the reaction rate constant amplification ratio with the temperature fluctuation

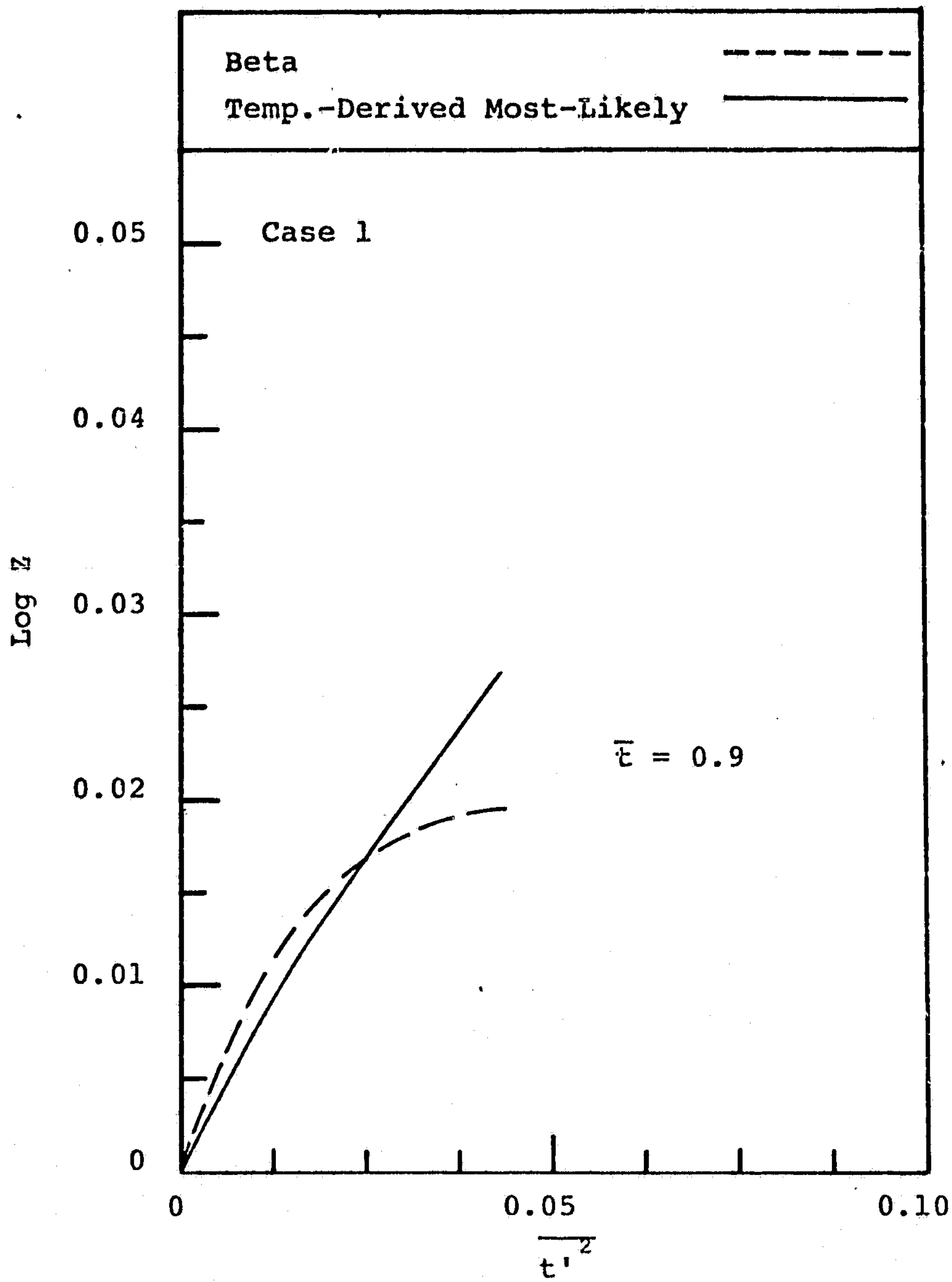


Figure 7. Variation of the reaction rate constant amplification ratio with the temperature fluctuation

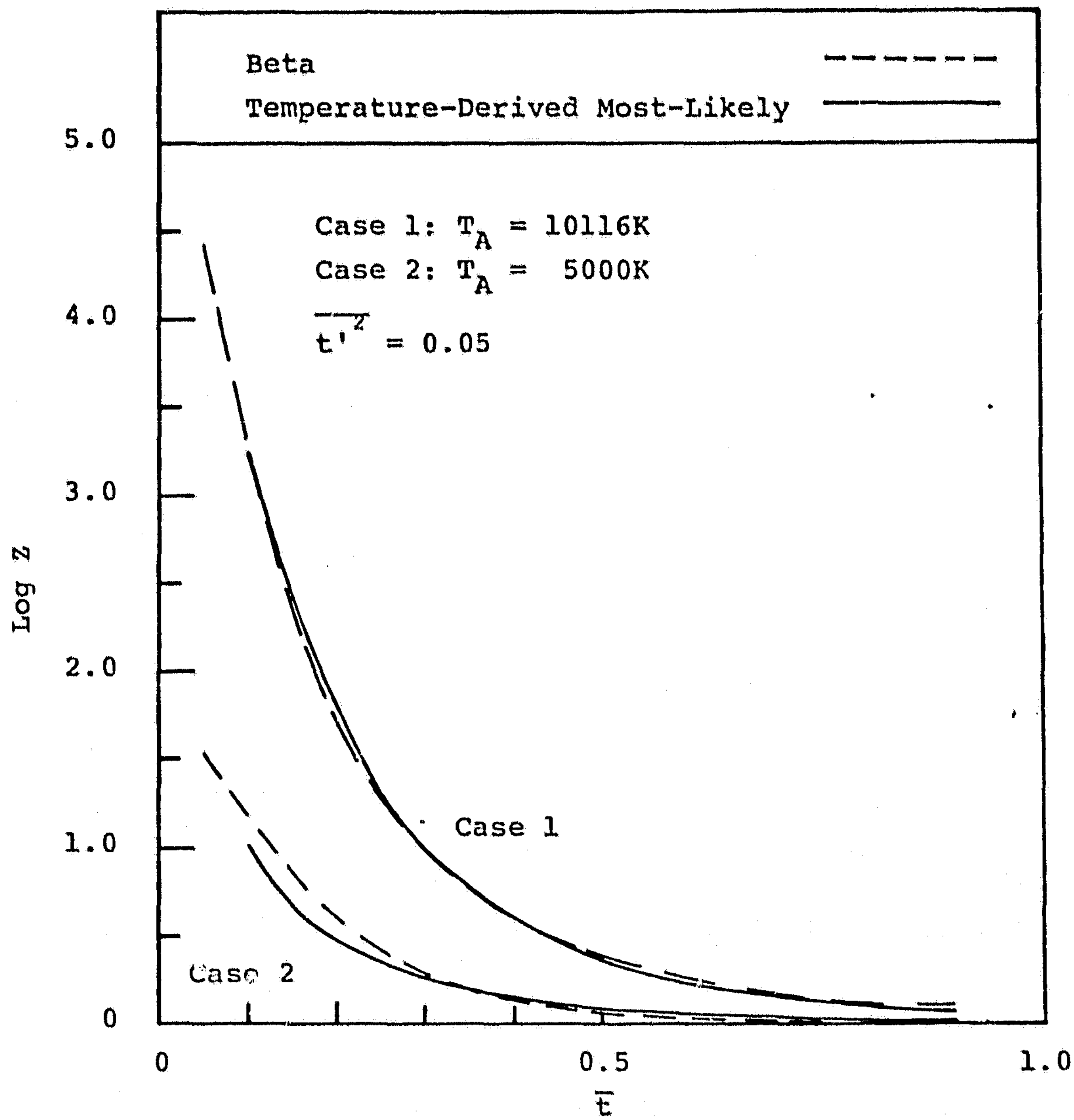


Figure 8. Variation of the reaction rate constant amplification ratio with activation temperature

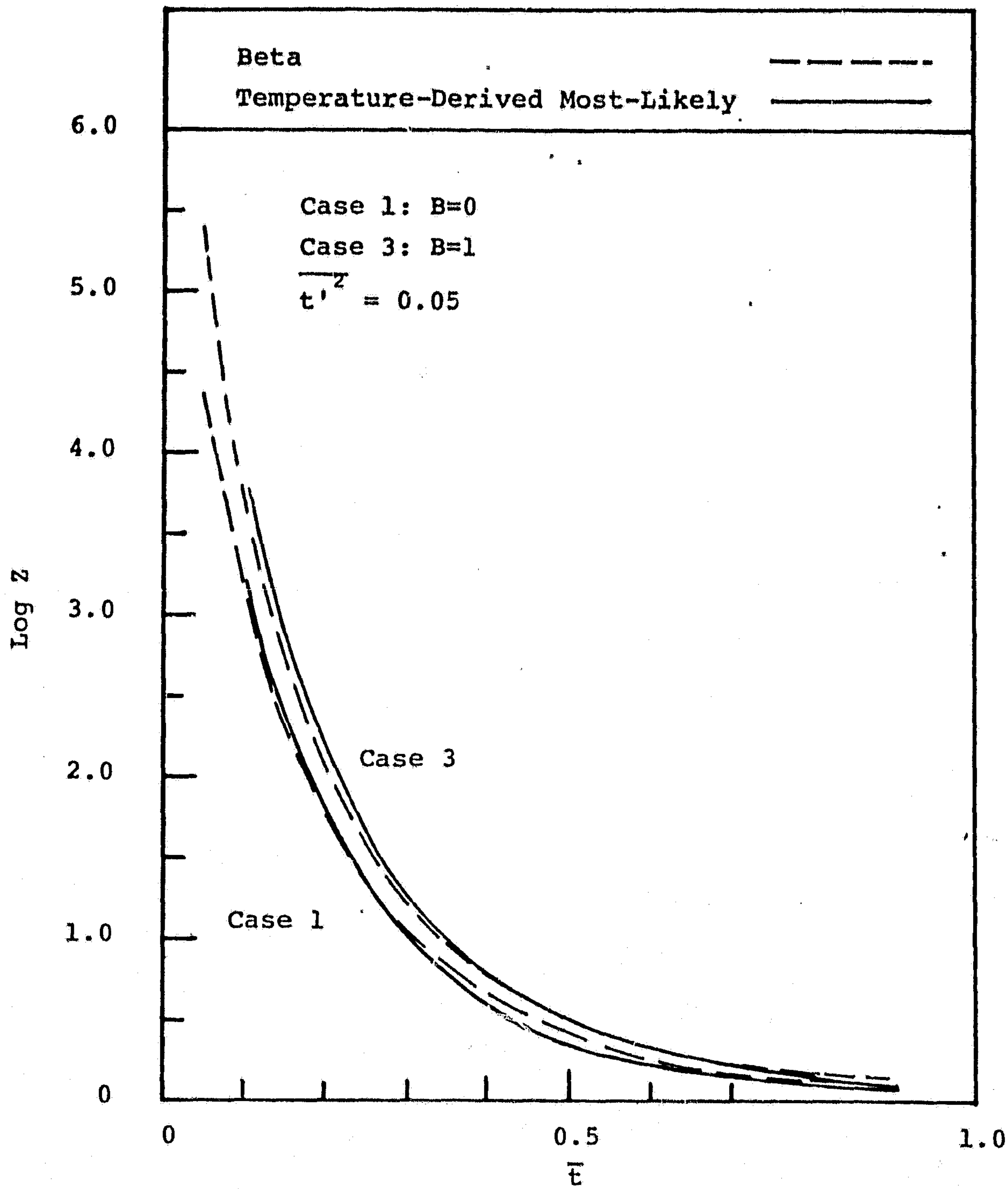


Figure 9. Variation of the reaction rate constant amplification ratio with temperature exponent, "B"

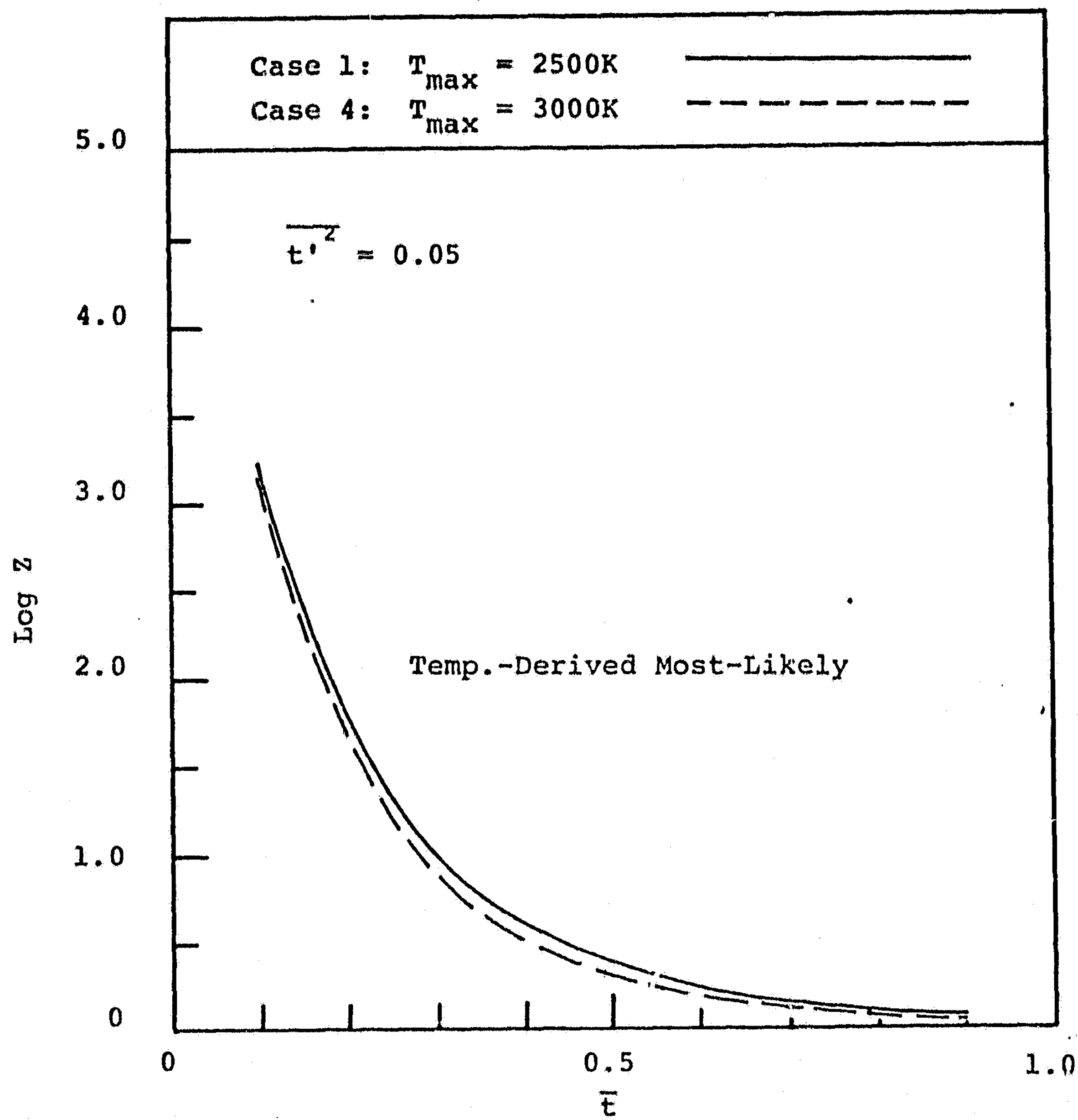


Figure 10. Variation of the reaction rate constant amplification ratio with the maximum temperature

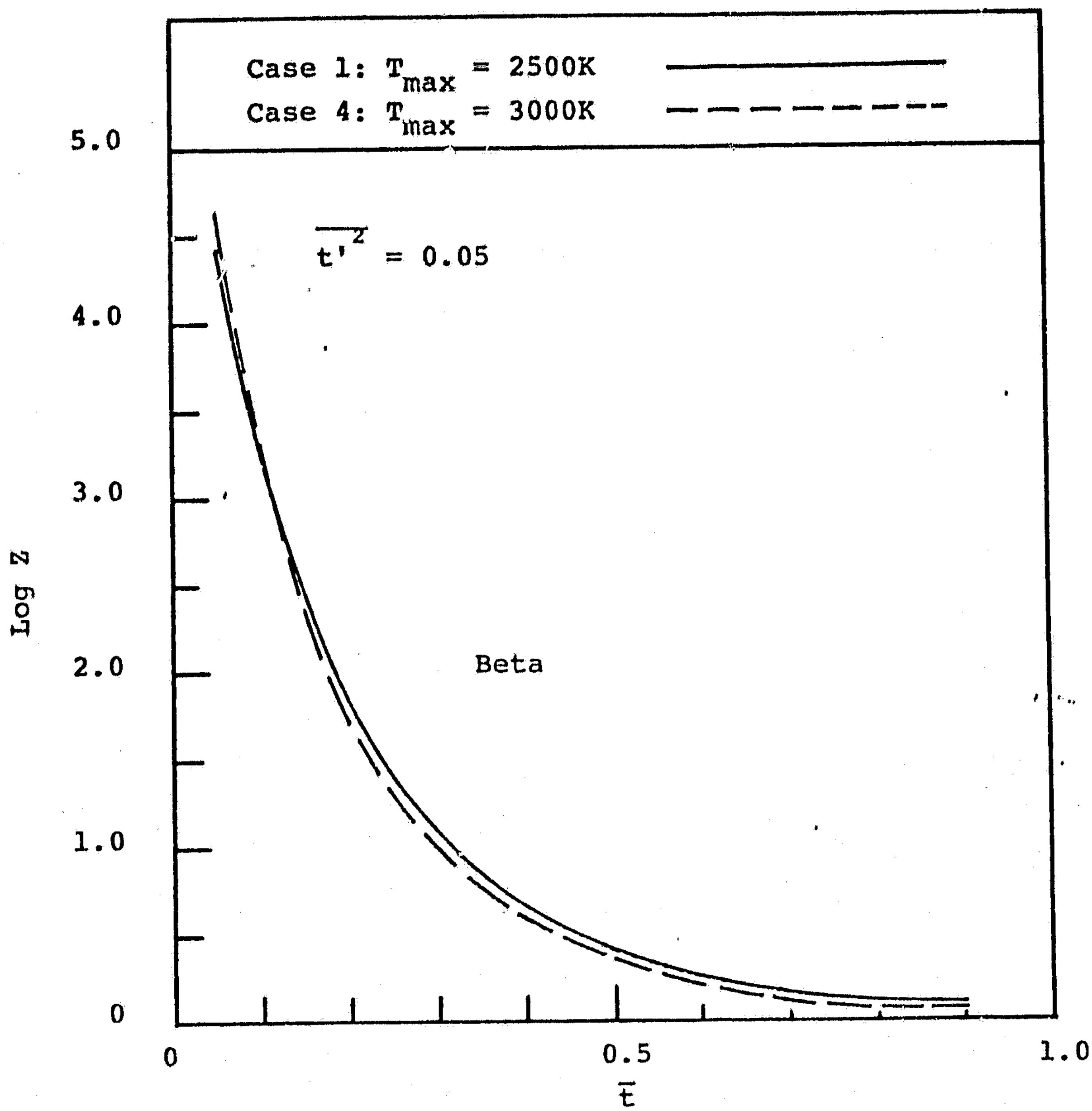


Figure 11. Variation of the reaction rate constant amplification ratio with the maximum temperature

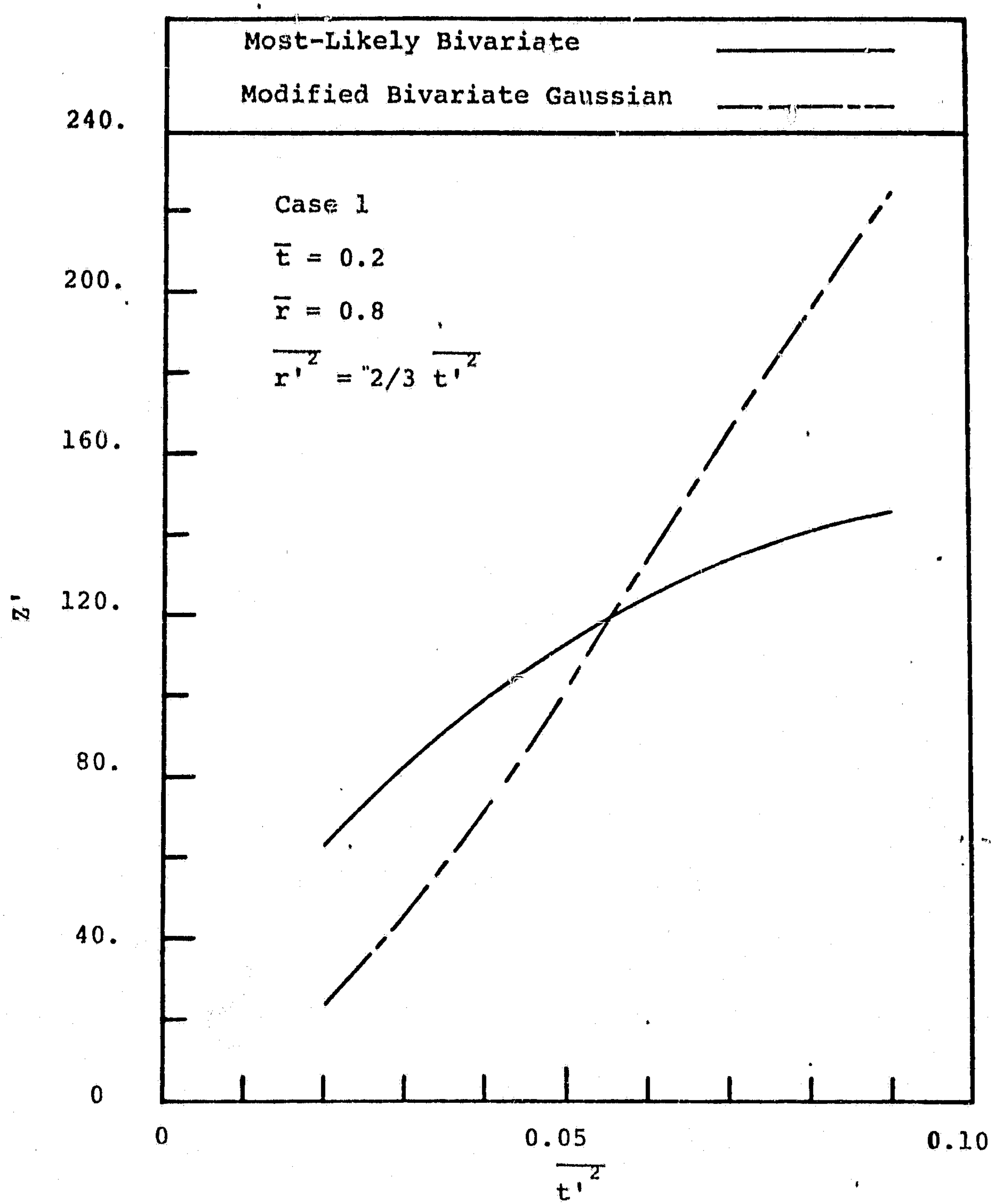


Figure 12. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the most-likely bivariate pdf and the modified bivariate Gaussian pdf

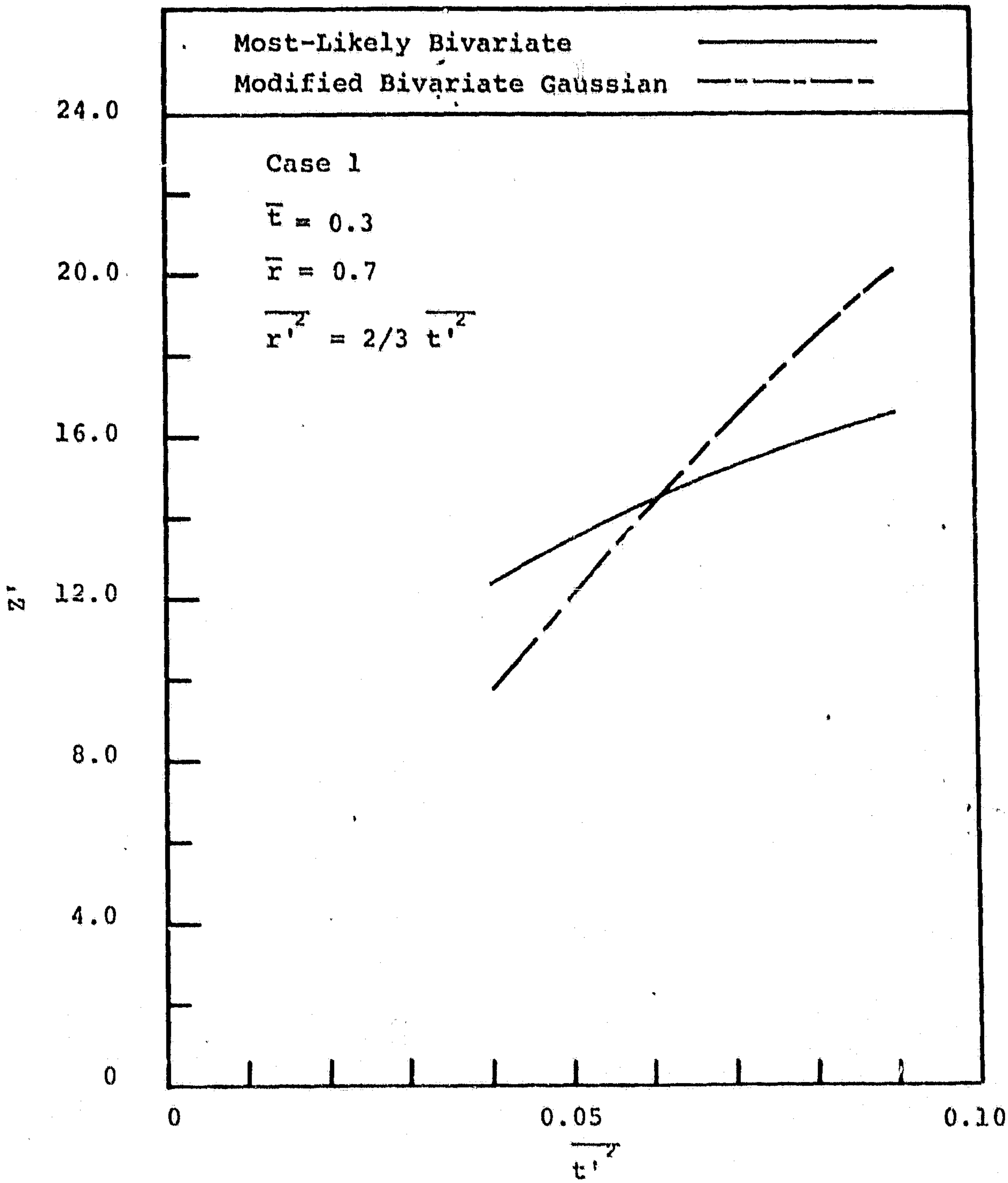


Figure 13. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the most-likely bivariate pdf and the modified bivariate Gaussian pdf

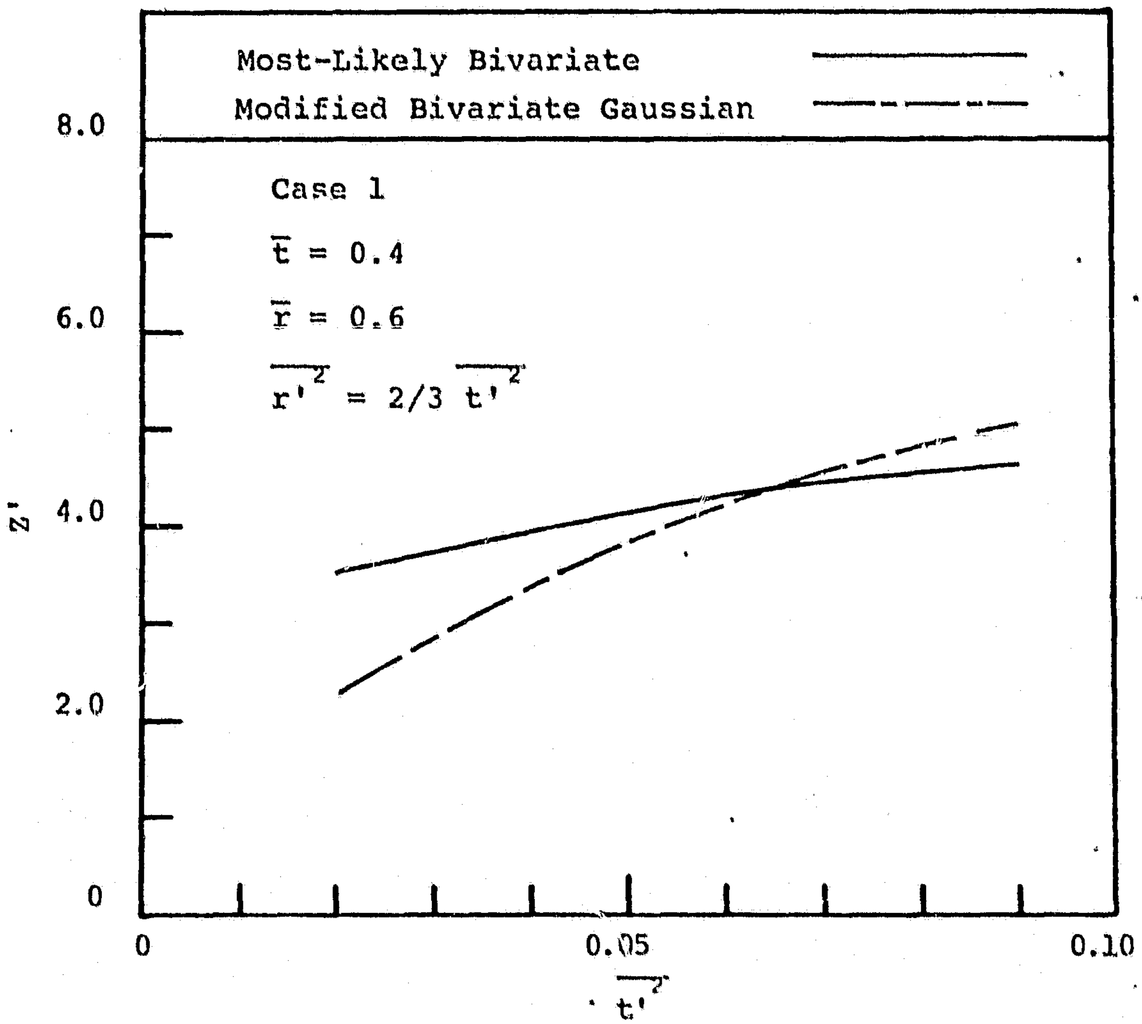


Figure 14. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the most-likely bivariate pdf and the modified bivariate Gaussian pdf

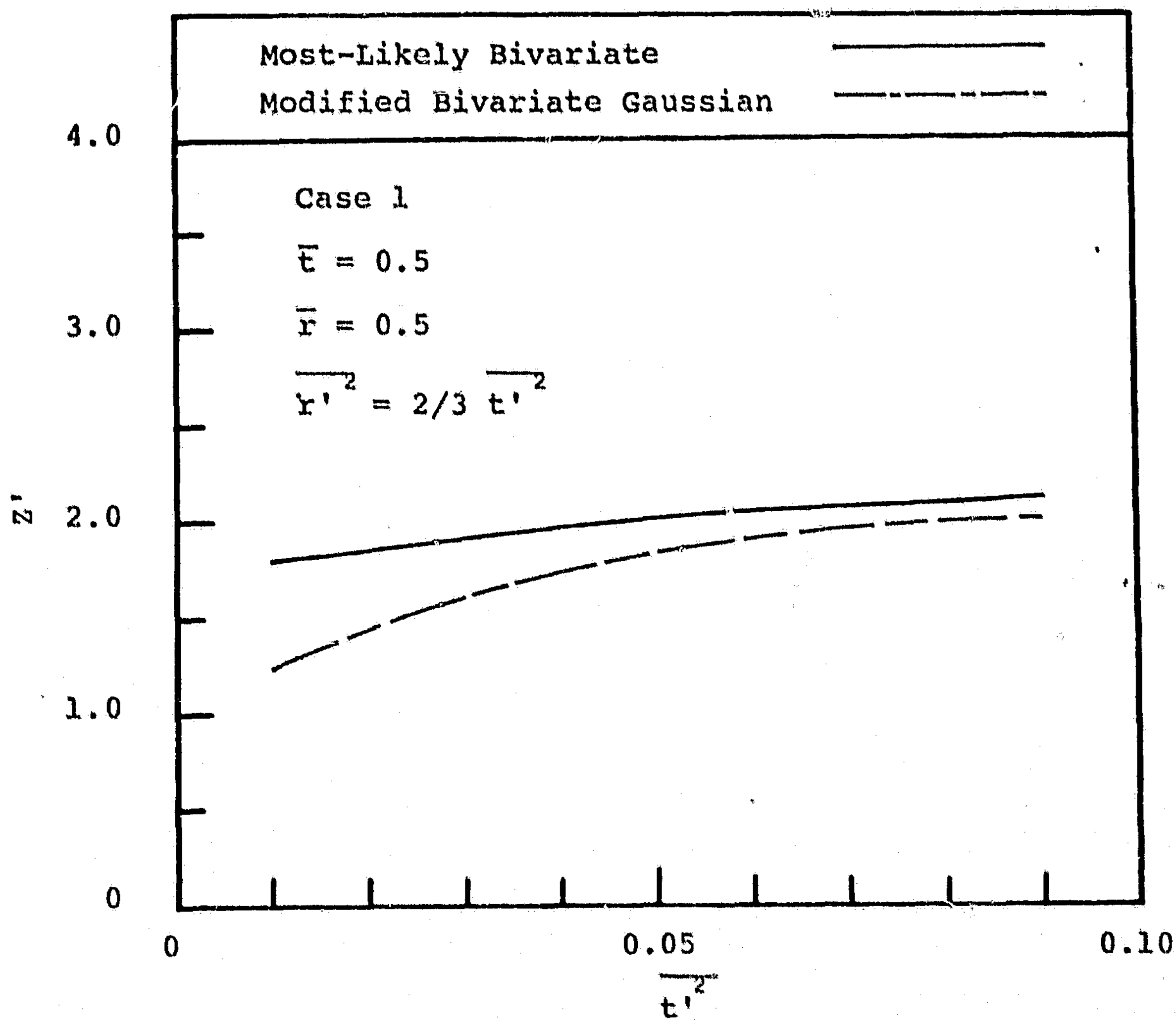


Figure 15. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the most-likely bivariate pdf and the modified bivariate Gaussian pdf

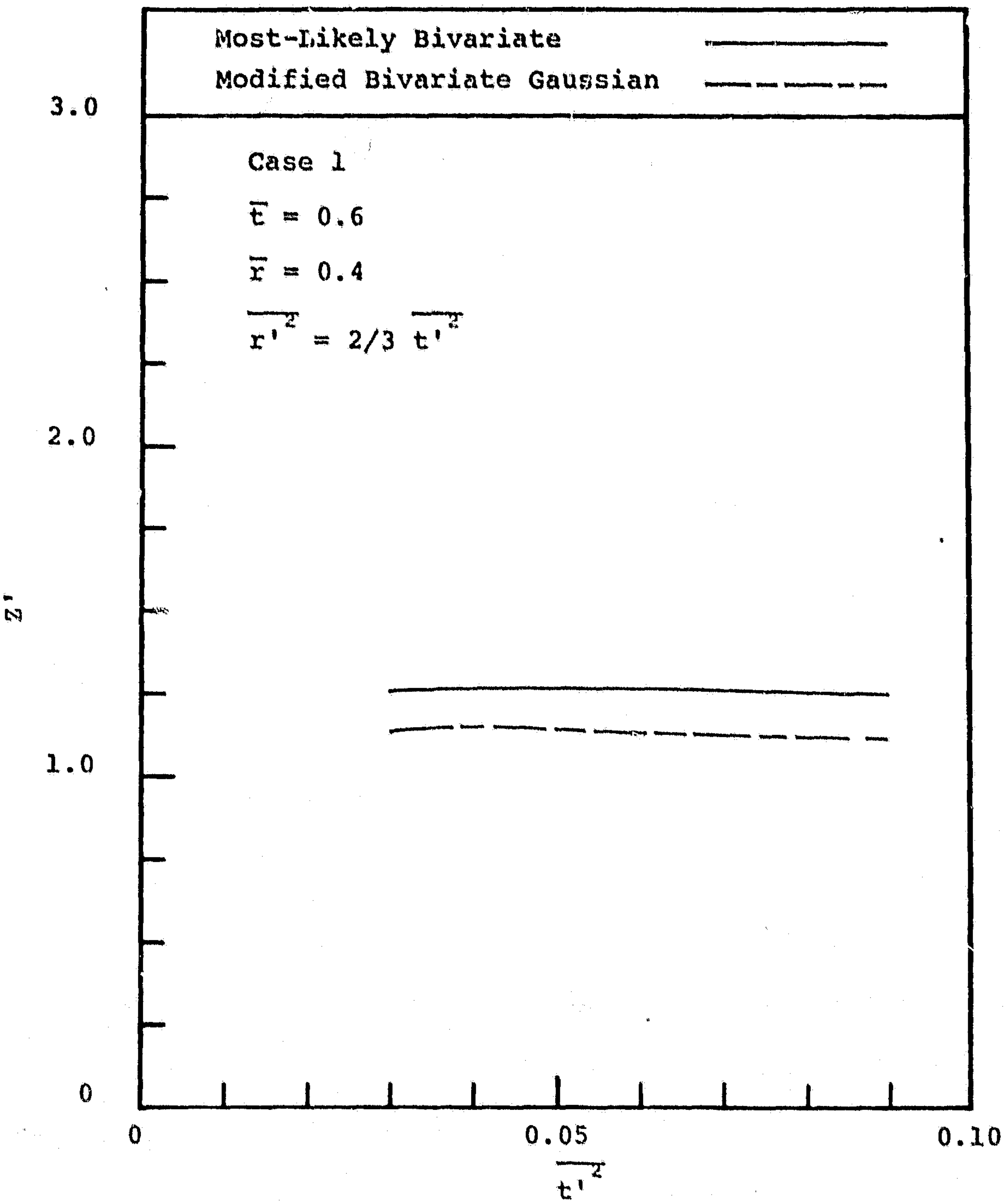


Figure 16. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the most-likely bivariate pdf and the modified bivariate Gaussian pdf

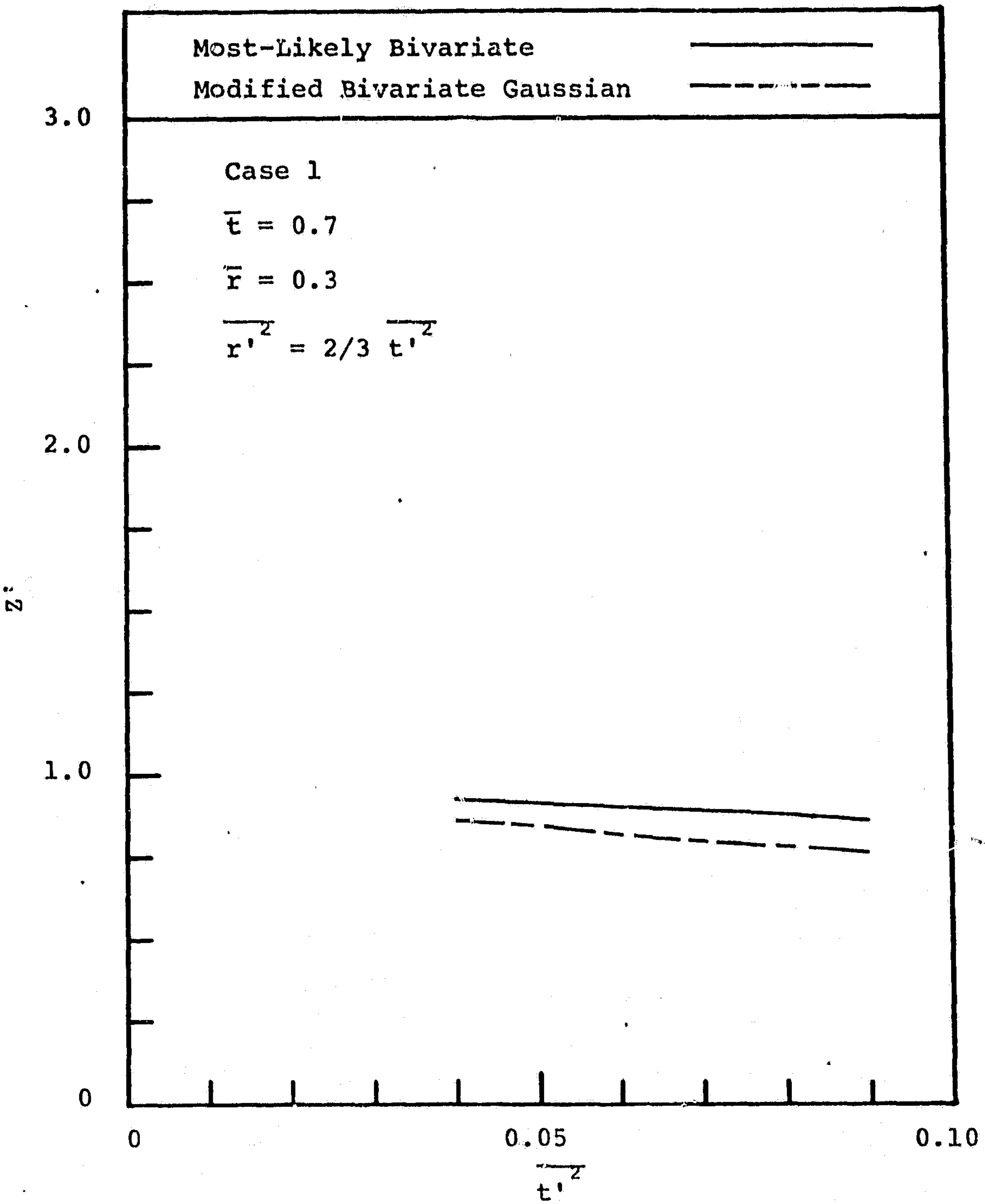


Figure 17. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the most-likely bivariate pdf and the modified bivariate Gaussian pdf

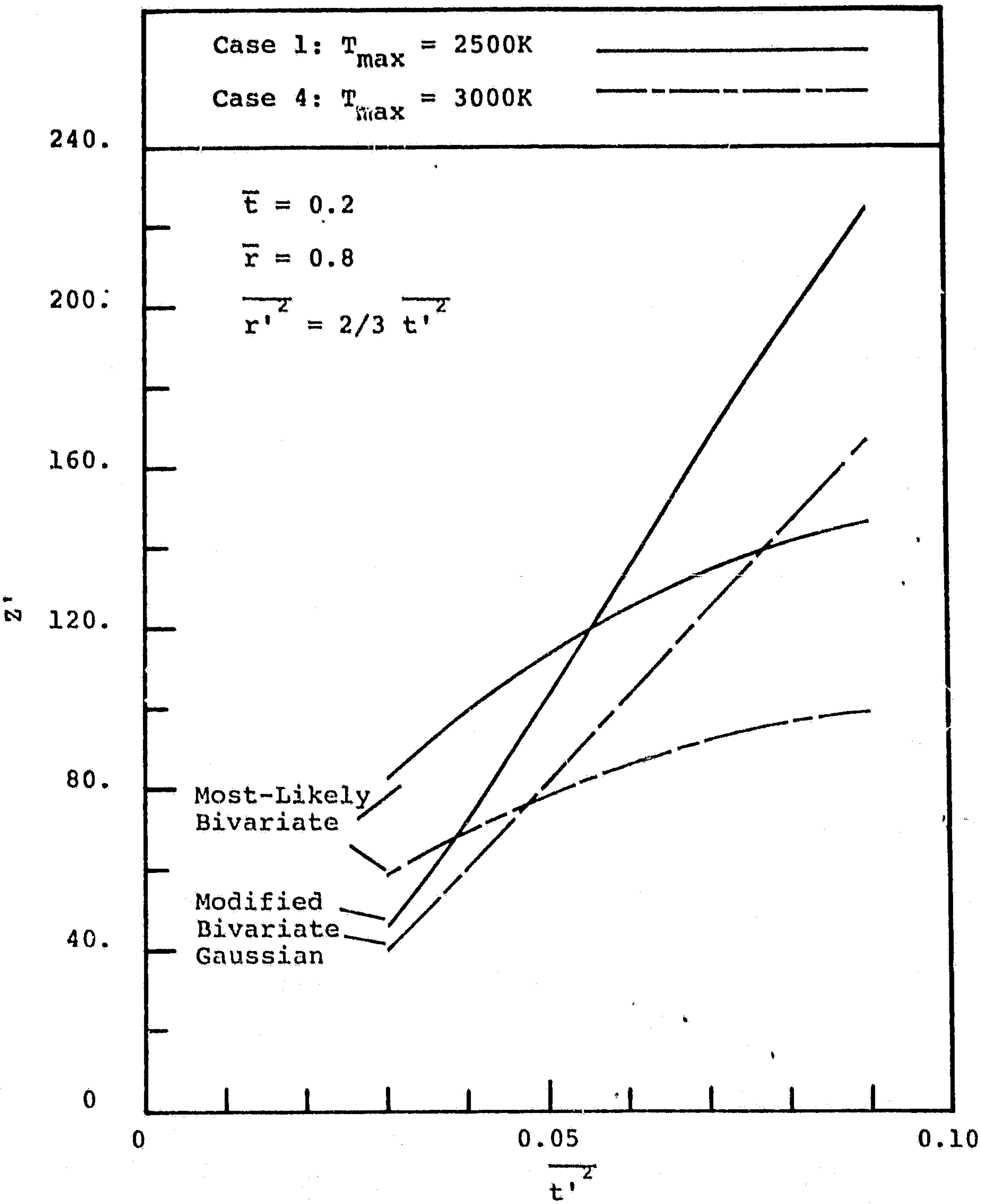


Figure 18. Variation of the reaction rate amplification ratio with the maximum temperature for the most-likely bivariate pdf and the modified bivariate Gaussian pdf

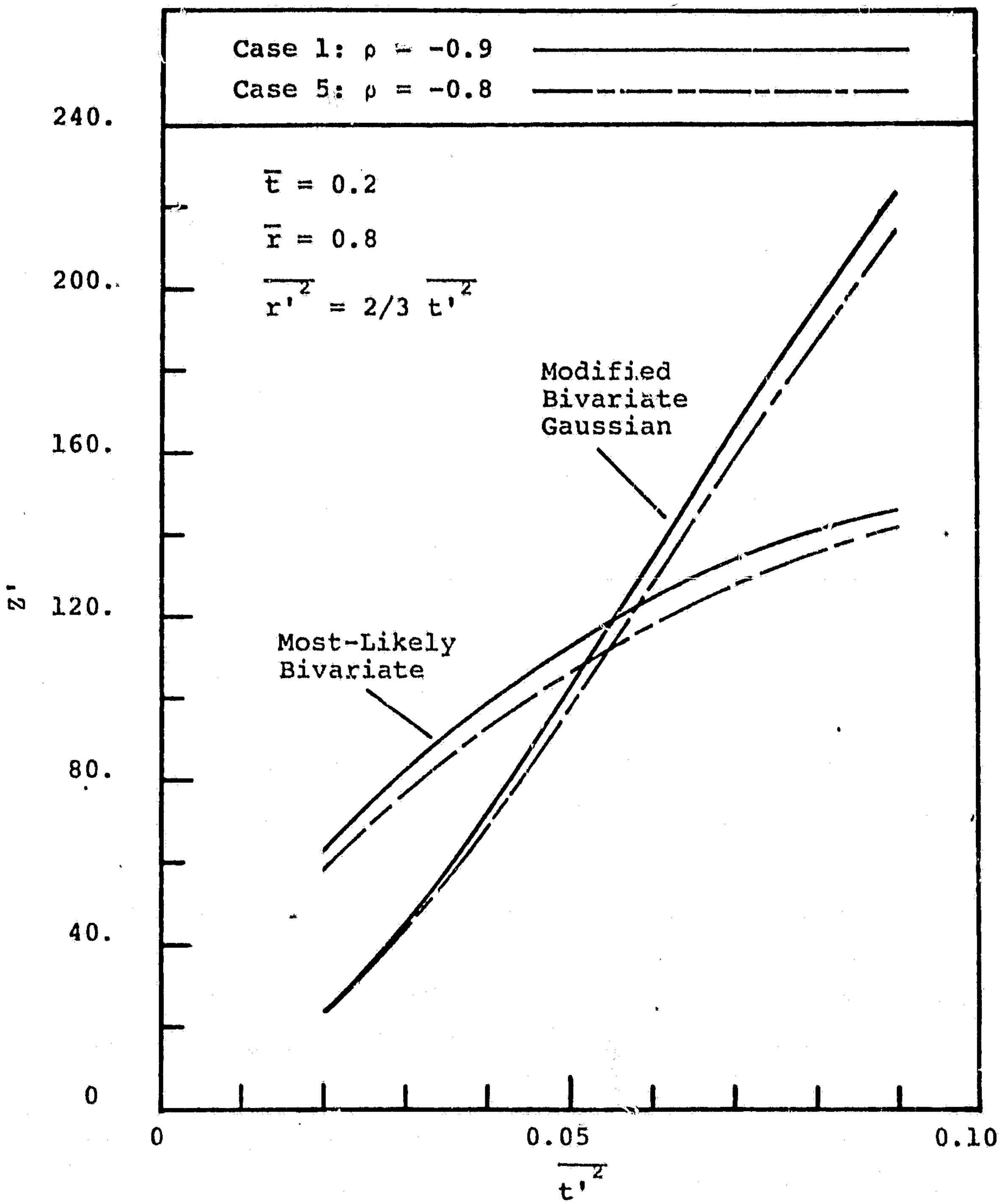


Figure 19. Variation of the reaction rate amplification ratio with the correlation coefficient for the most-likely bivariate pdf and the modified bivariate Gaussian pdf

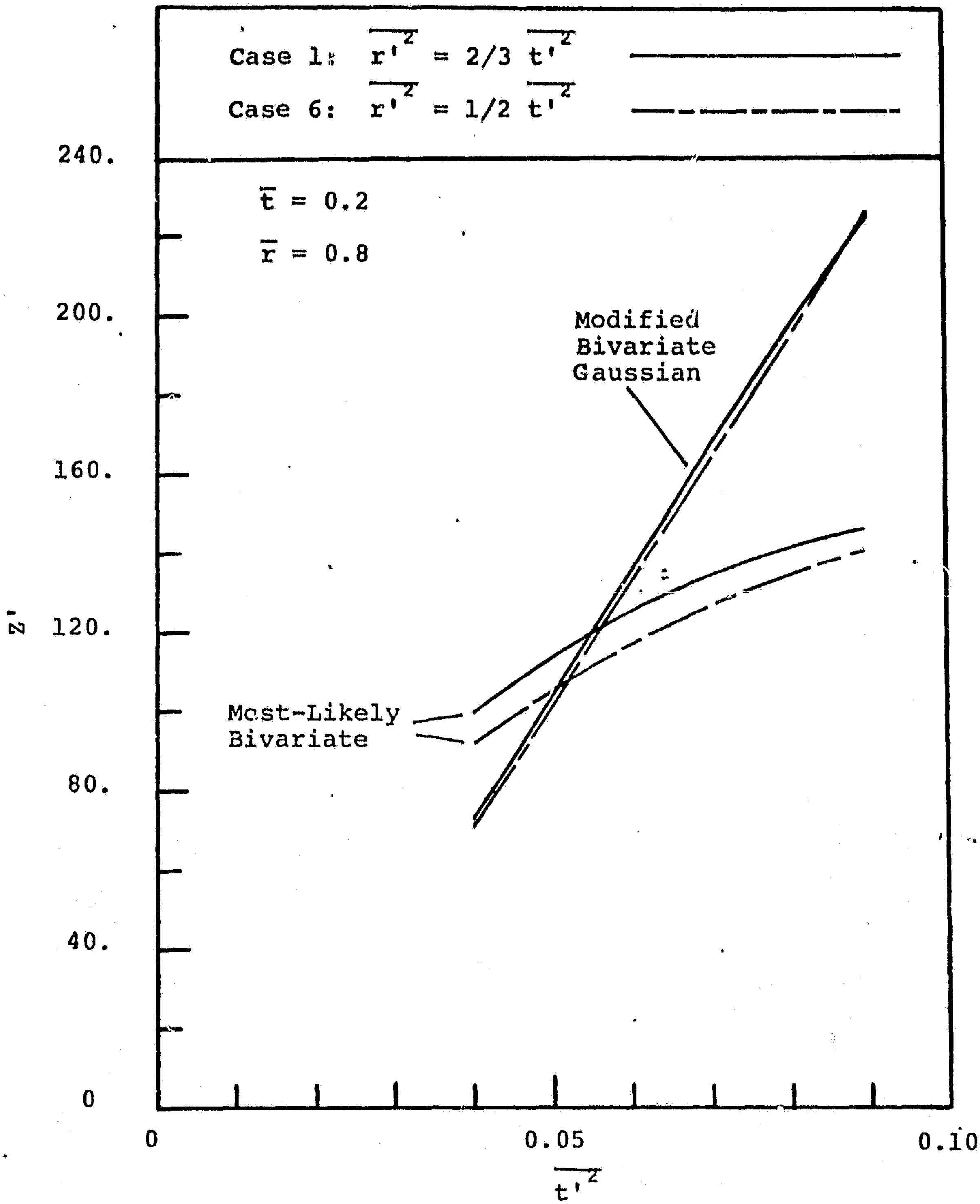


Figure 20. Variation of the reaction rate amplification ratio with the relationship between temperature and species fluctuations for the most-likely bivariate pdf and the modified bivariate Gaussian pdf

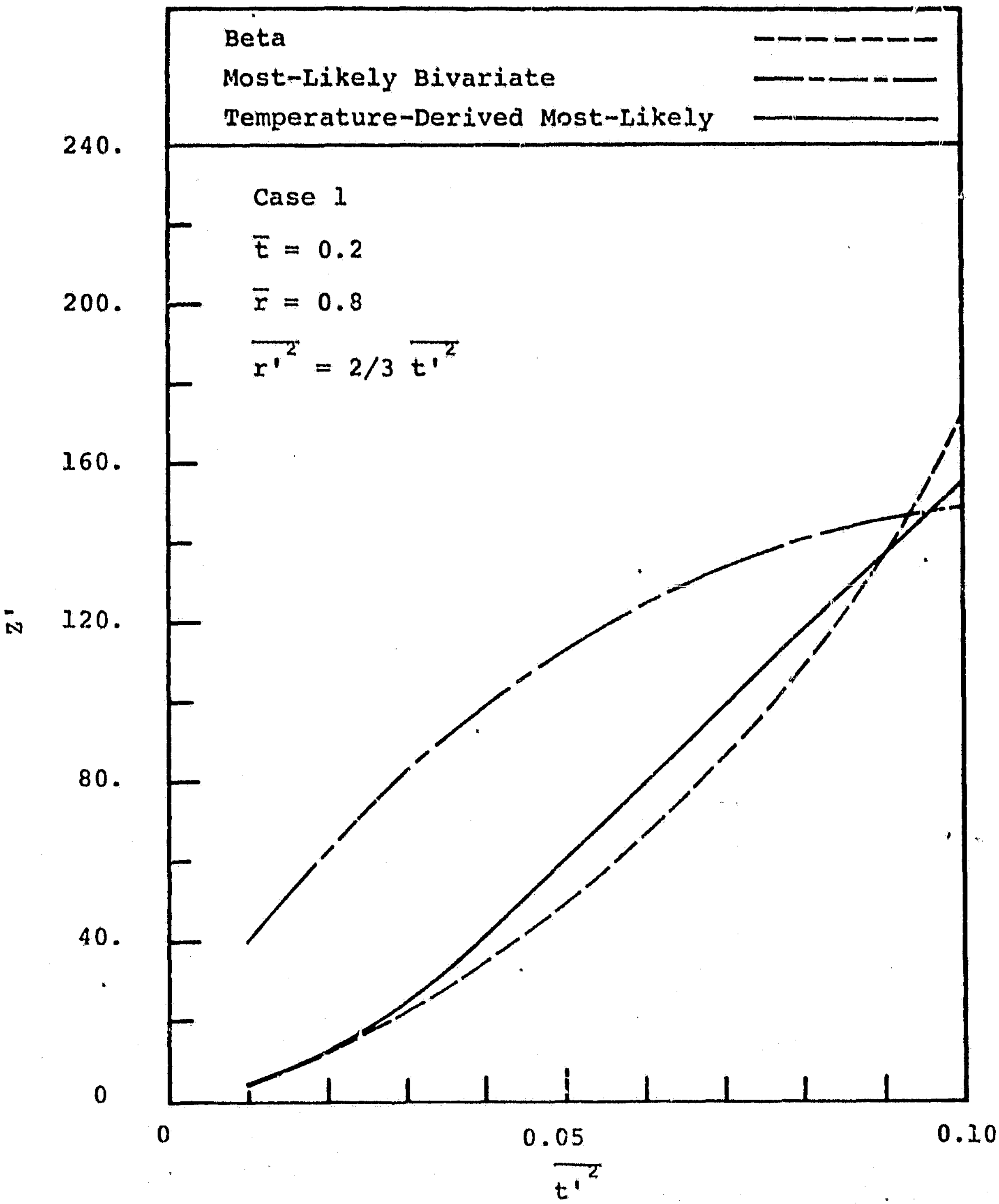


Figure 21. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the beta pdf, most-likely bivariate pdf, and the temperature-derived most-likely pdf

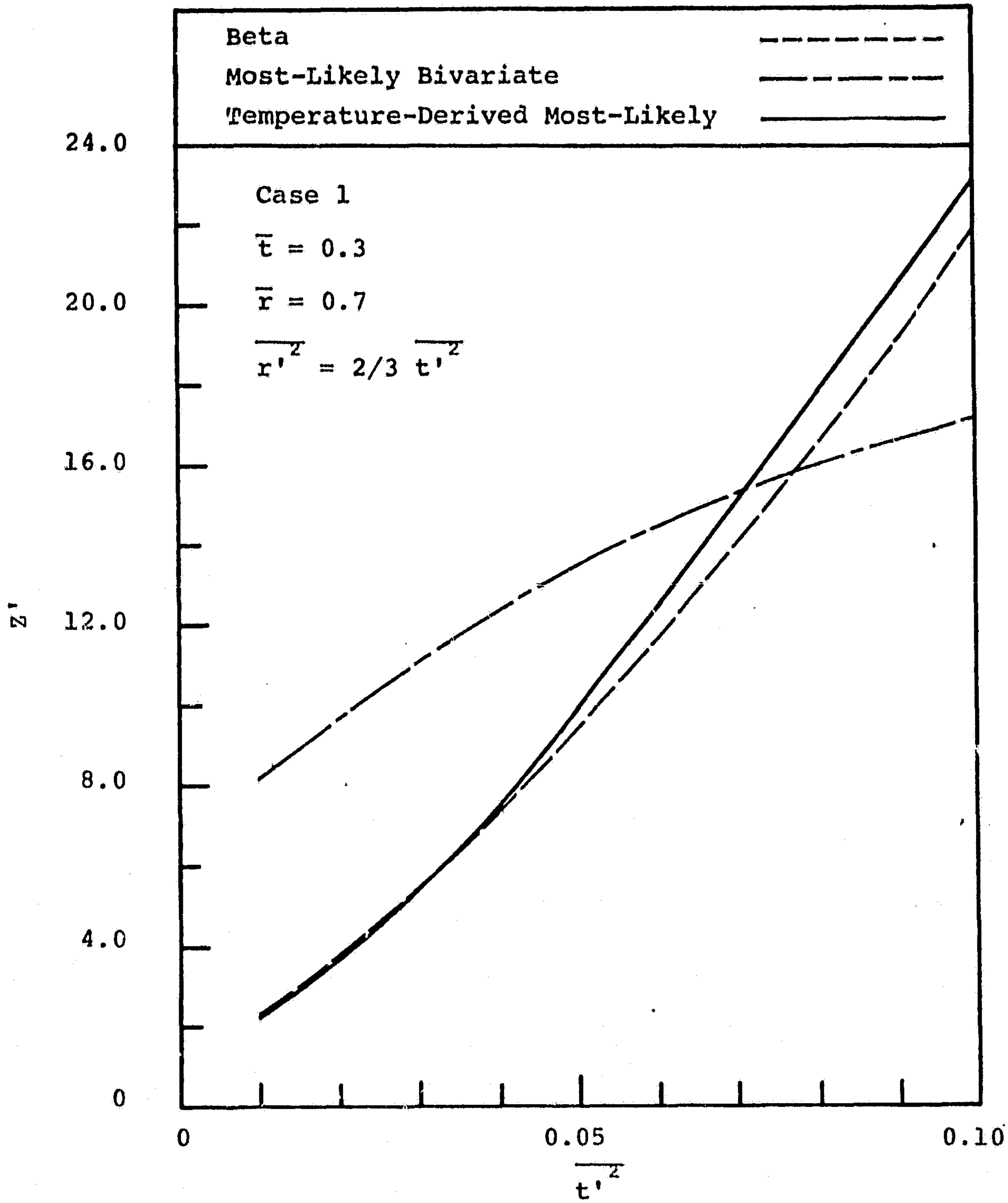


Figure 22. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the beta pdf, most-likely bivariate pdf, and the temperature-derived most-likely pdf

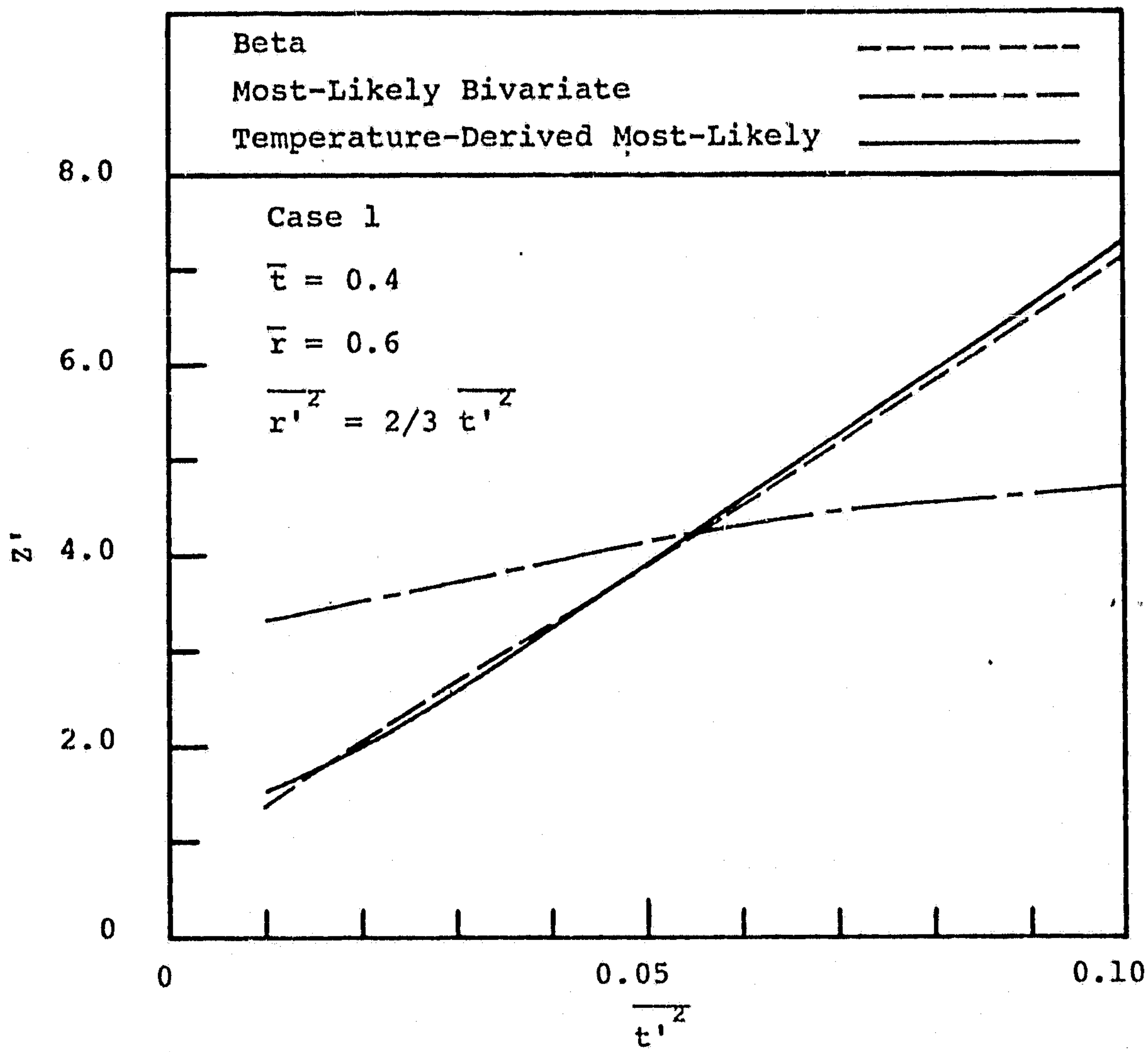


Figure 23. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the beta pdf, most-likely bivariate pdf, and the temperature-derived most-likely pdf

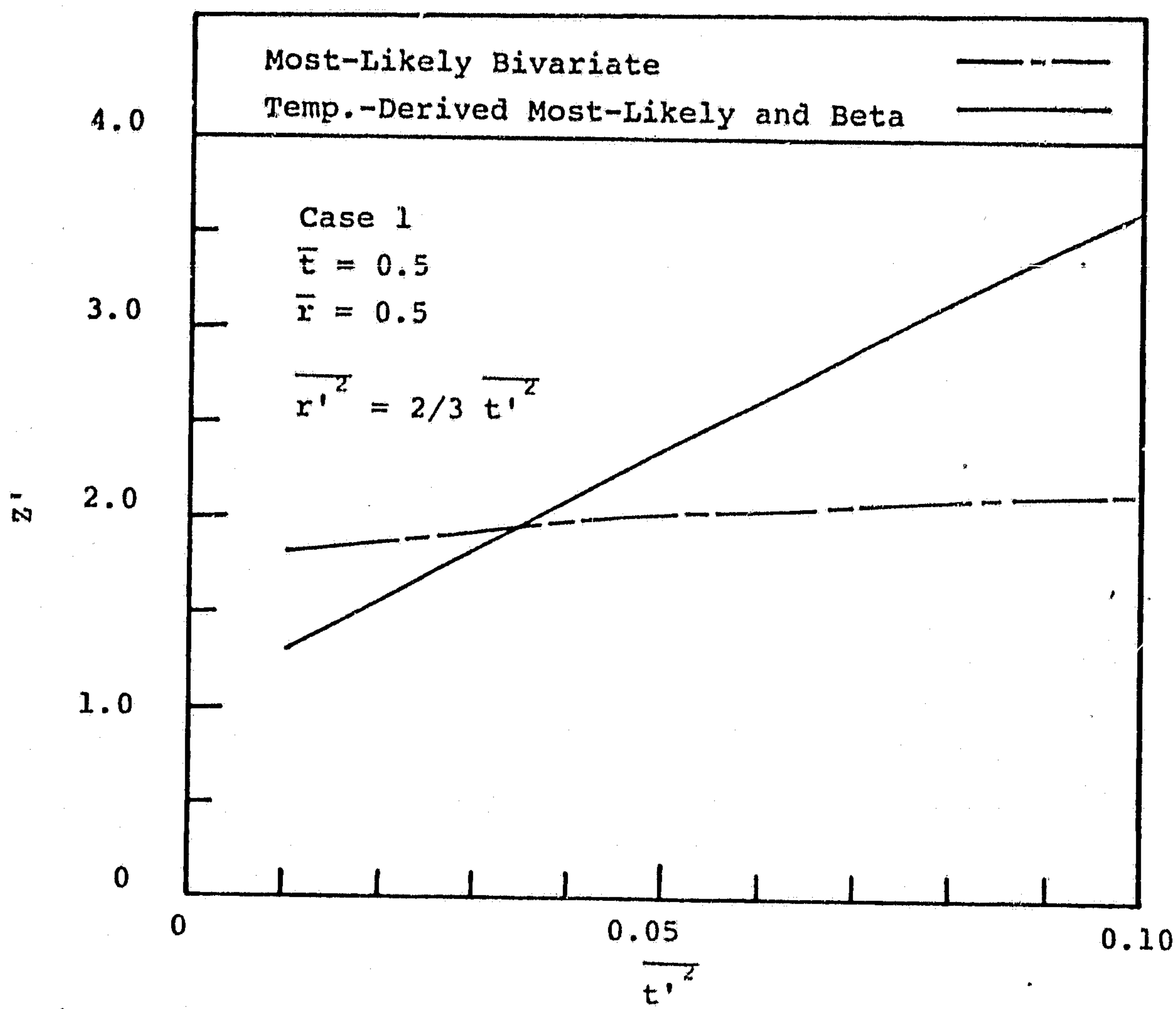


Figure 24. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the beta pdf, most-likely bivariate pdf, and the temperature-derived most-likely pdf

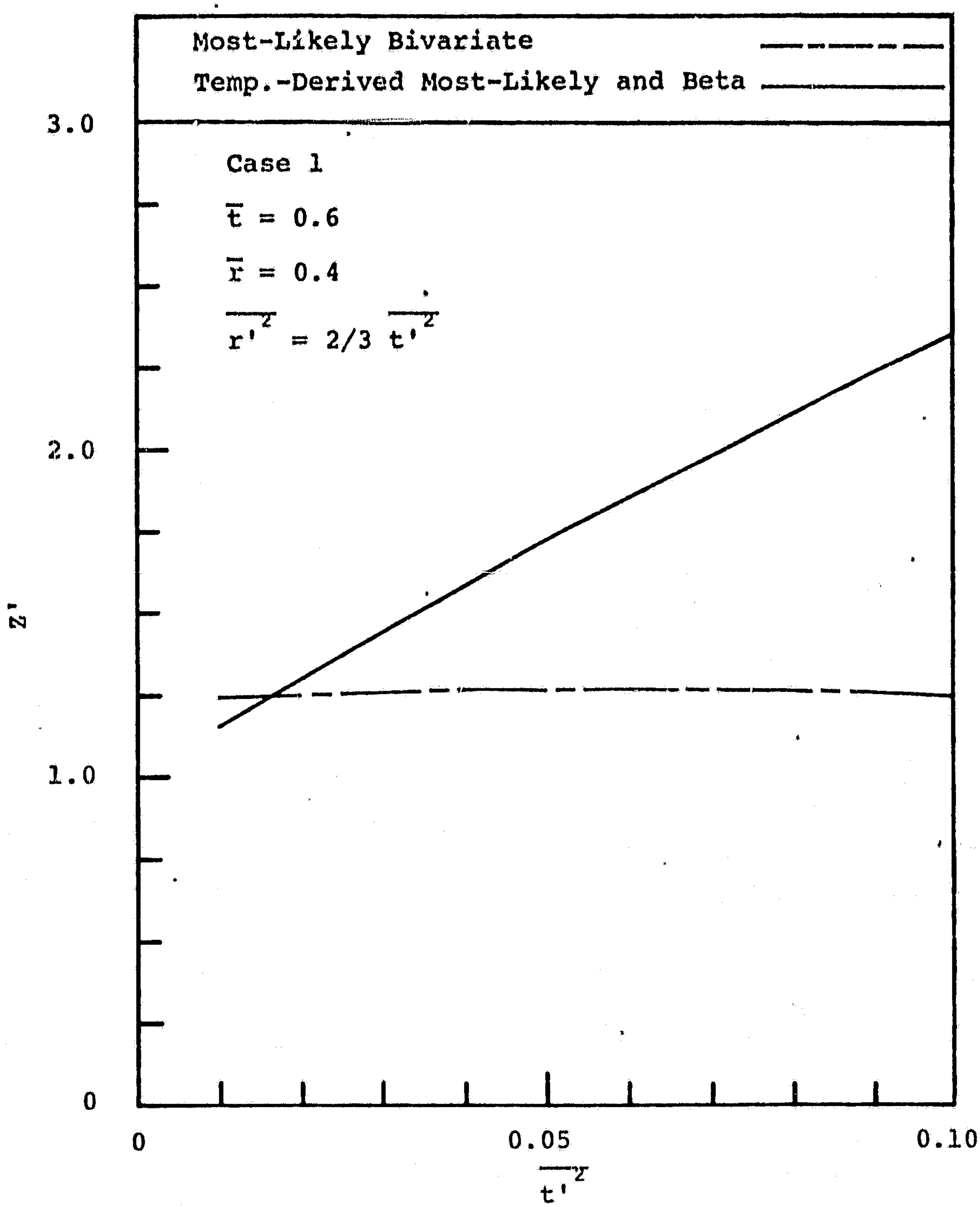


Figure 25. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the beta pdf, the most-likely bivariate pdf, and the temperature-derived most-likely pdf

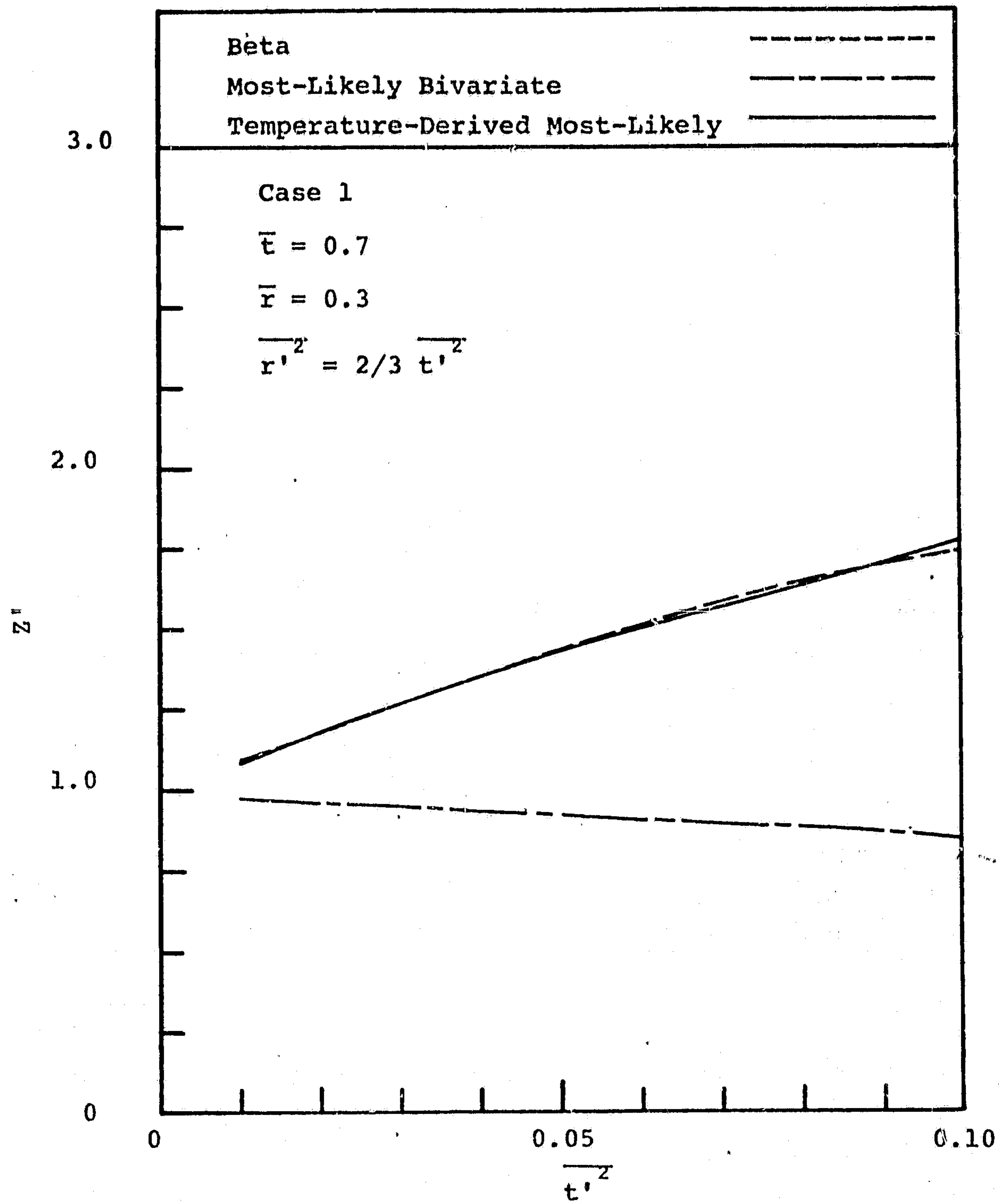
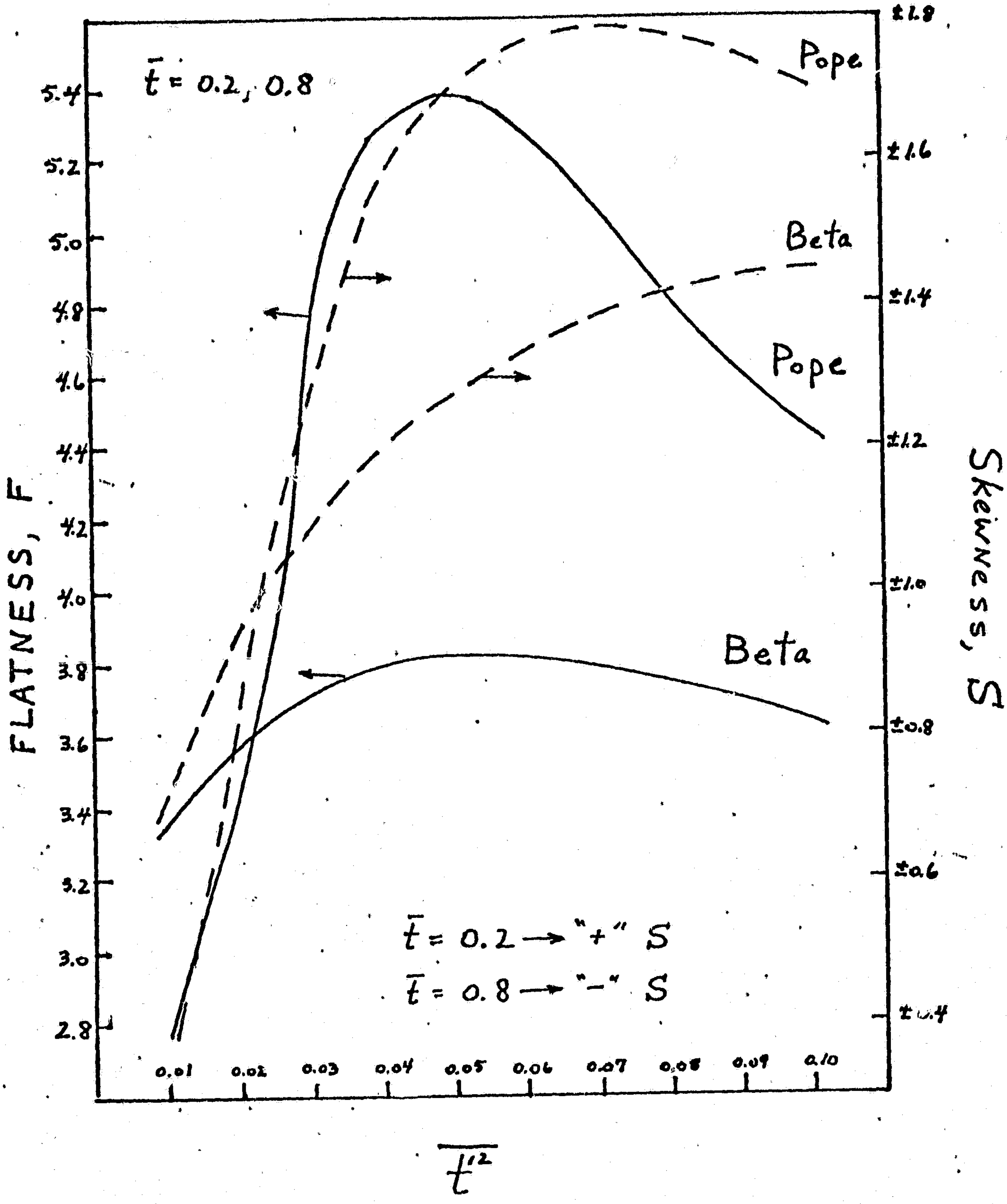


Figure 26. Variation of the reaction rate amplification ratio with temperature and species fluctuations for the beta pdf, the most-likely bivariate pdf, and the temperature-derived most-likely pdf



$\overline{t'^2}$

Figure 27 Skewness + flatness factor for Pope and Beta pdf's with $\bar{t}$ = 0.2 and 0.8.

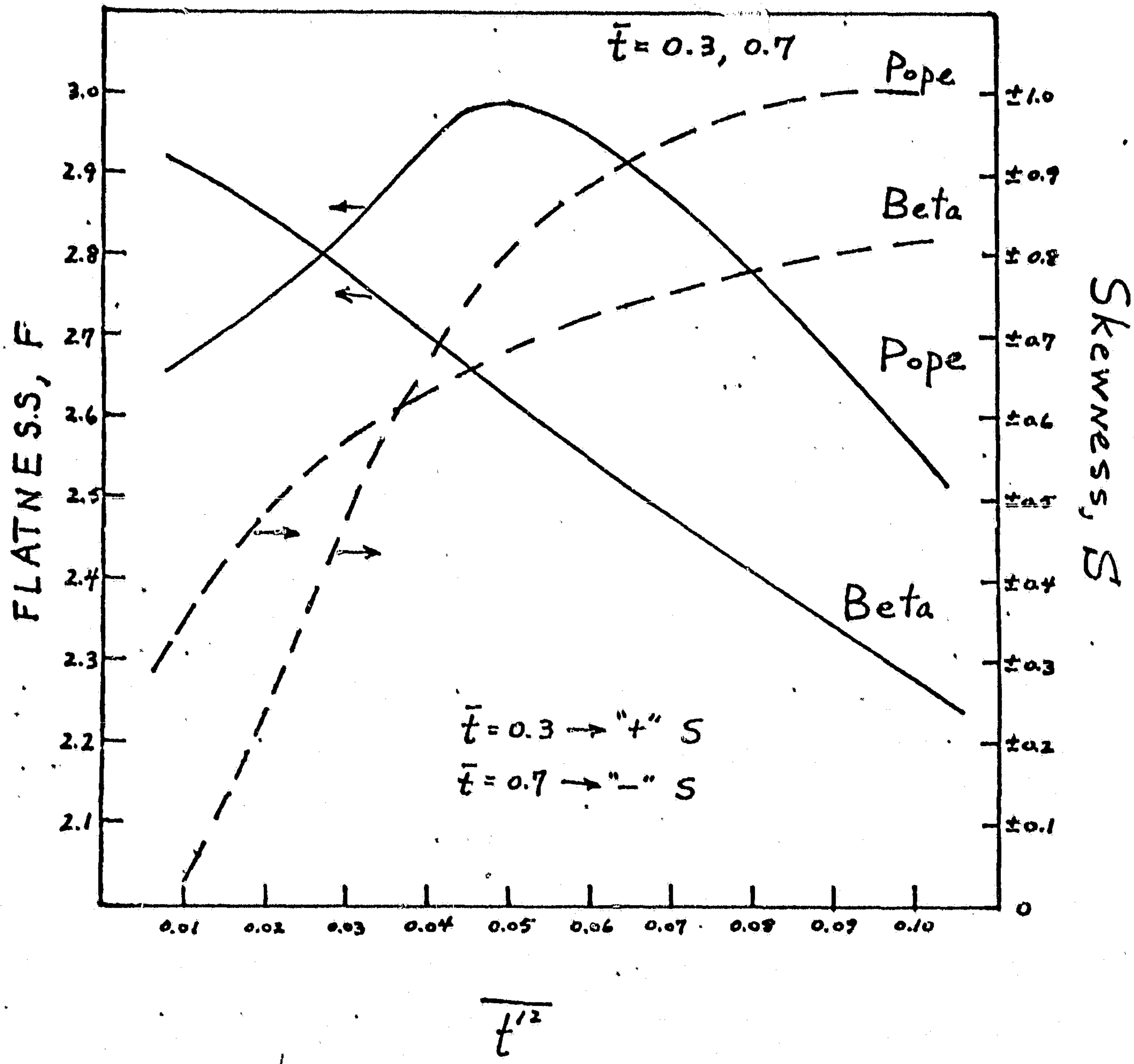


Figure 28 Skewness + flatness factor for Pope and Beta pdf's for $\bar{t}$ = 0.3 and 0.7.

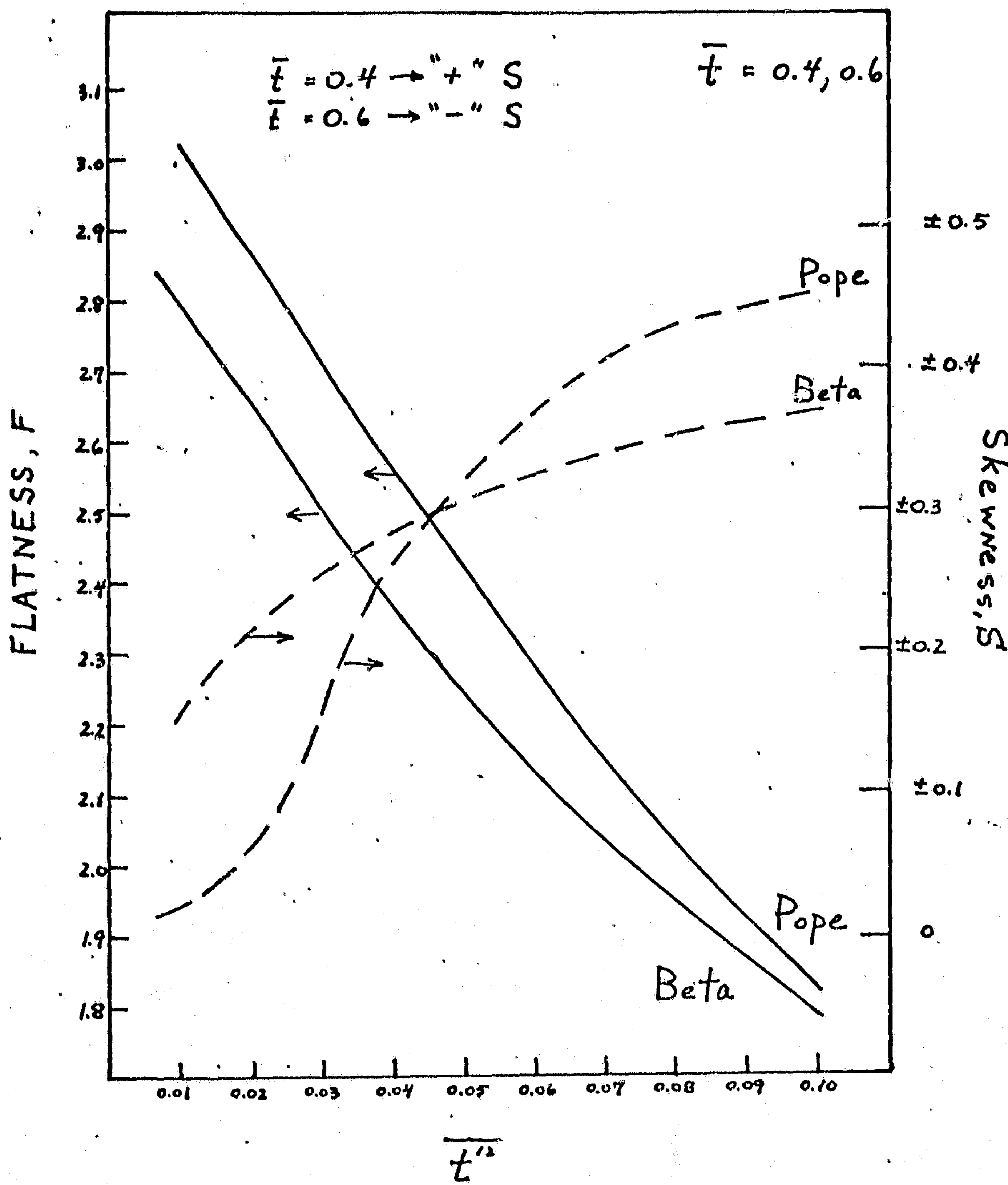


Figure 29 Skewness and flatness factors for the Pope and Beta pdf's with $\bar{t}$ = 0.4 and 0.6.

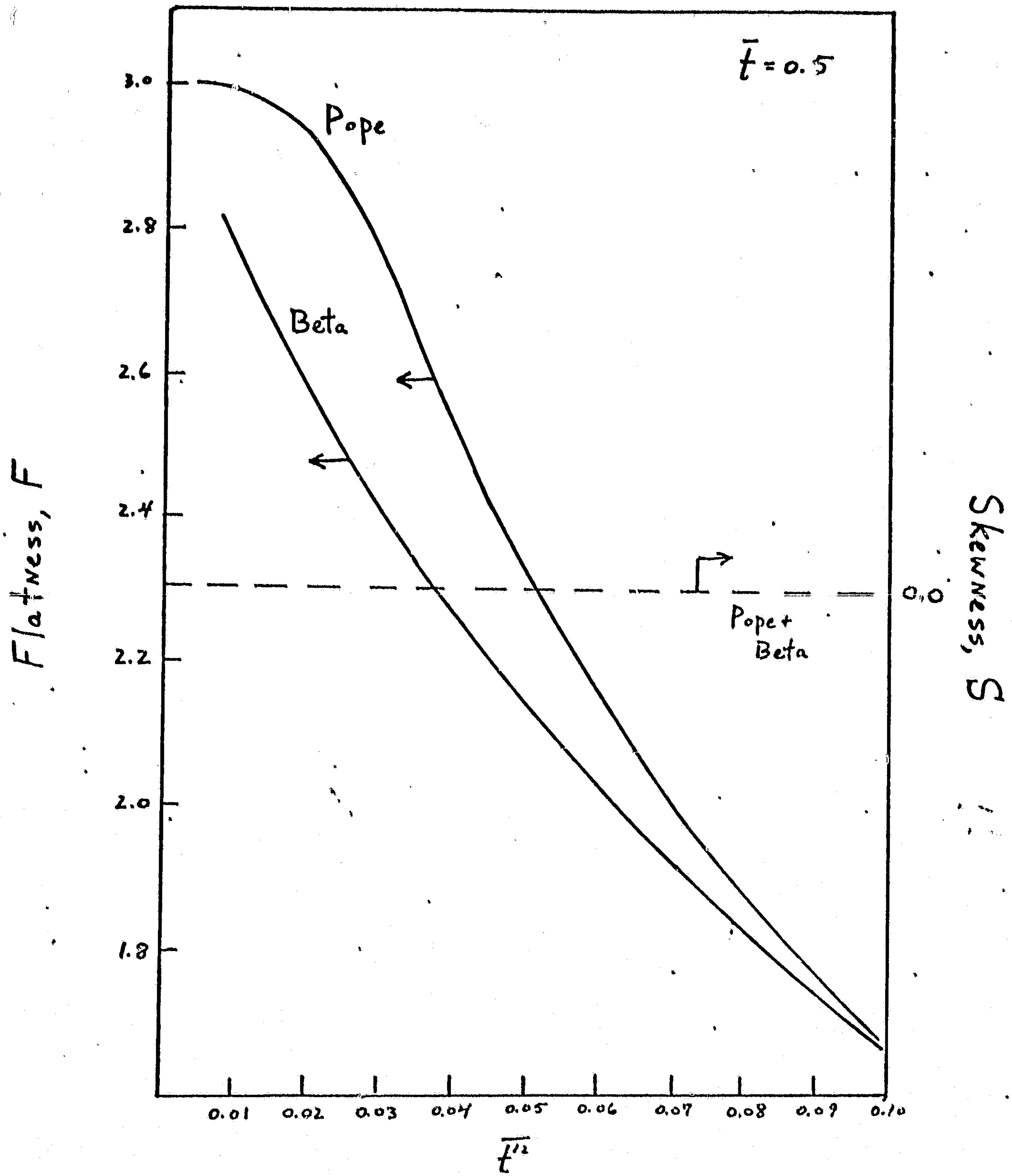


Figure 30 Skewness and flatness factors for the Pope and Beta pdf's with $\bar{t} = 0.5$.

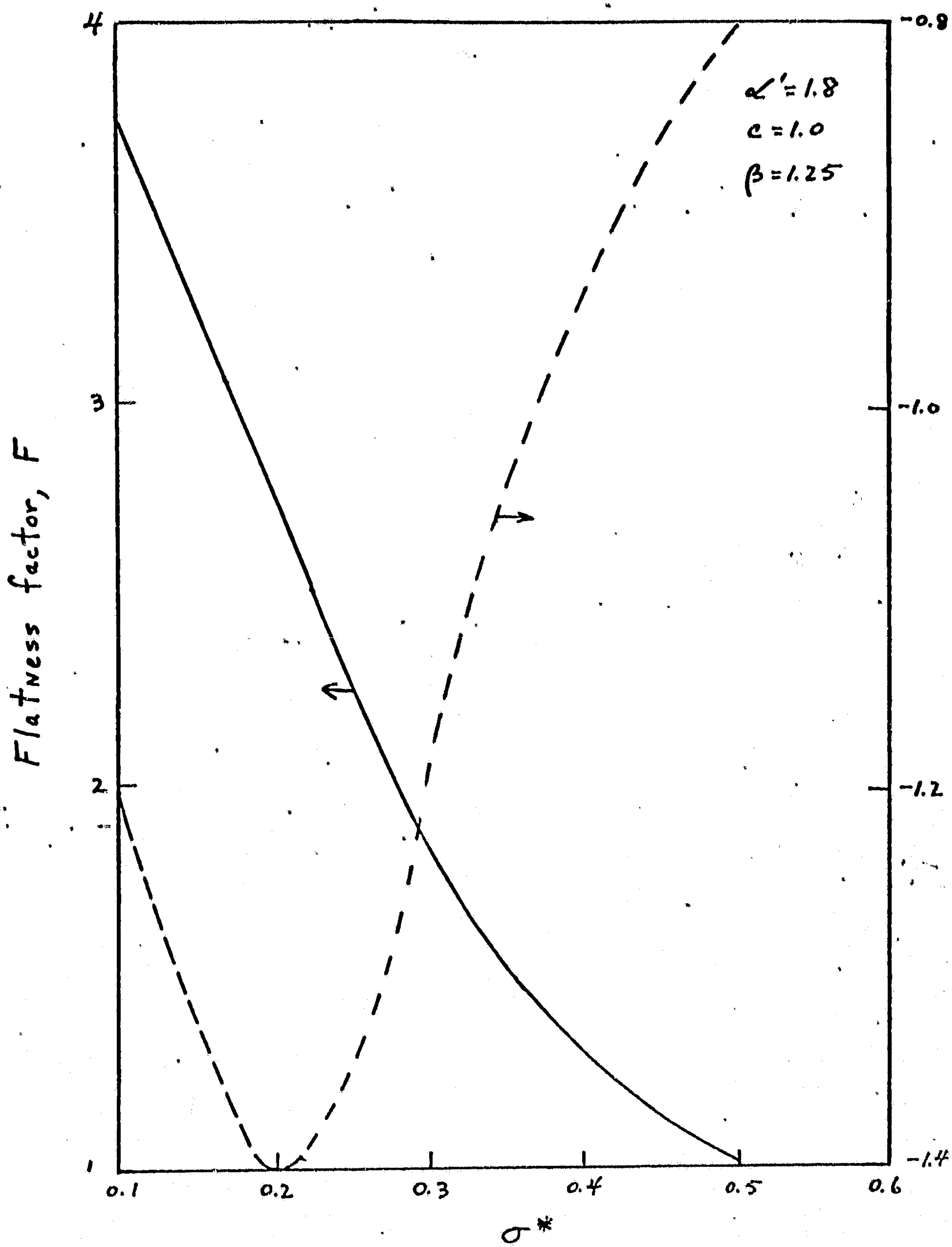


Figure 31: Flatness factor and skewness distributions for the Ramp pdf as a function of σ^*

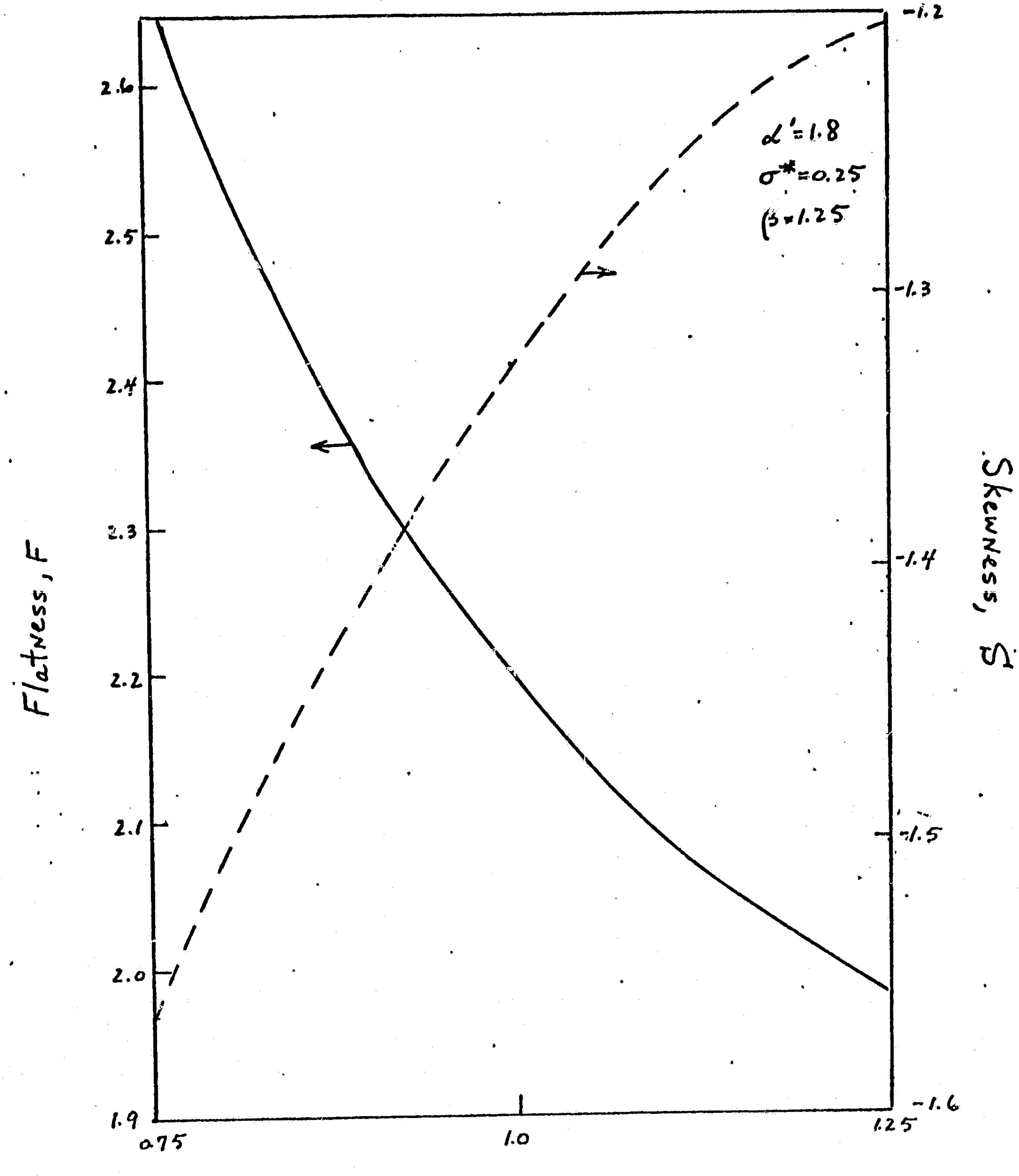


Figure 32 Flatness factor and skewness distributions for the Ramp pdf as a function of "c".

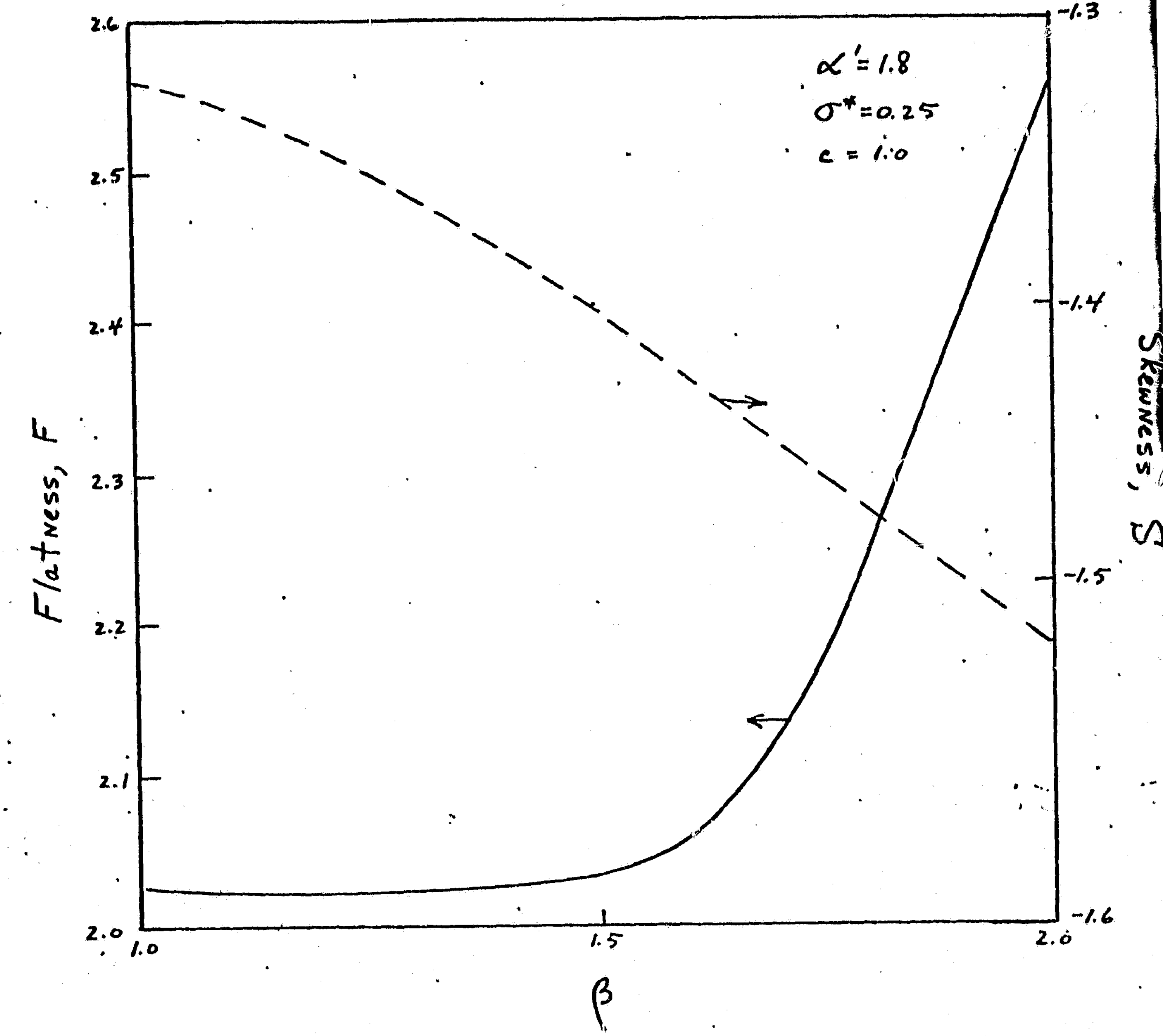


Figure 33: Flatness factor and skewness distributions for the Ramp pdf as a function of β.

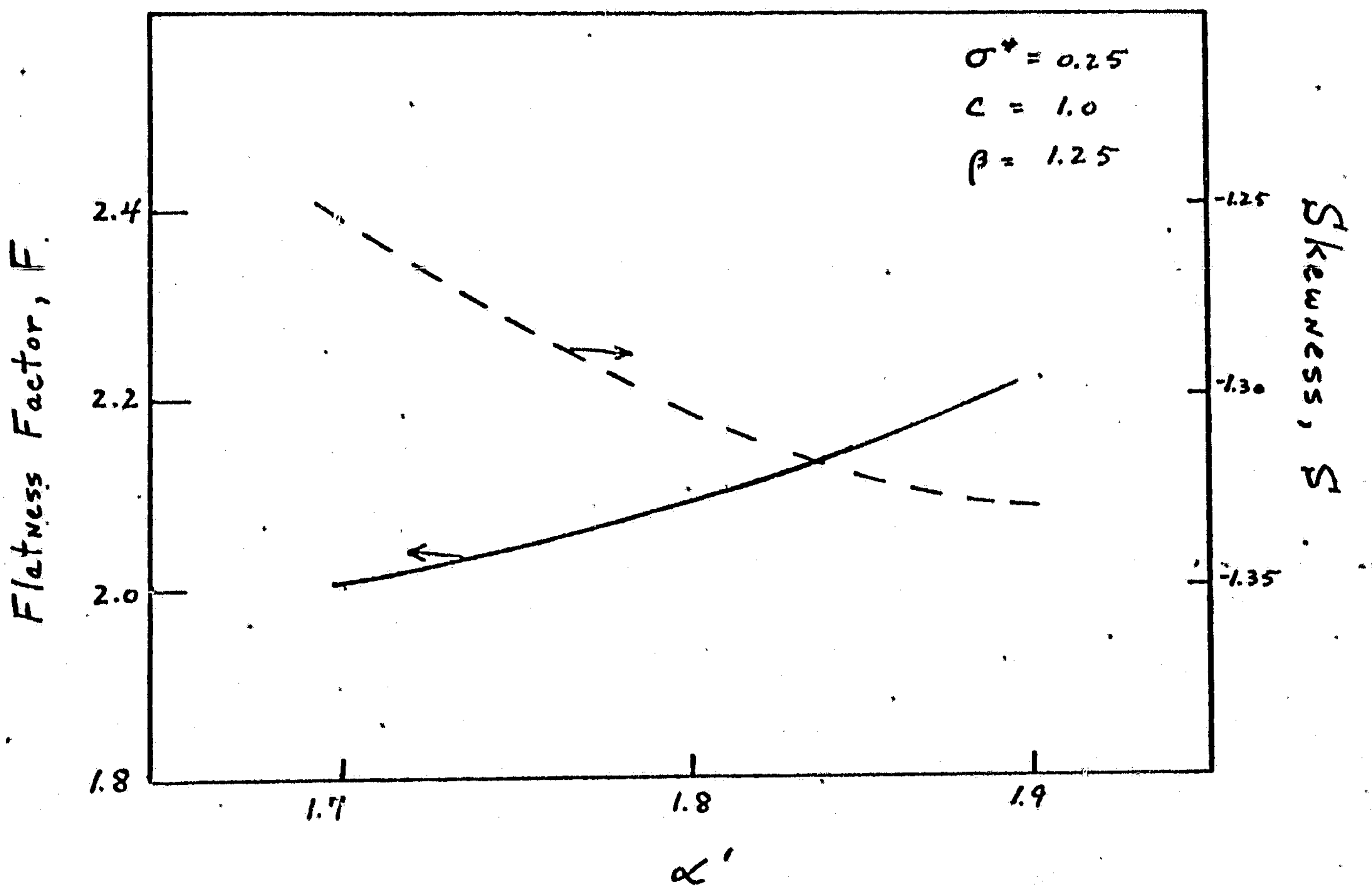


Figure 34. Flatness factor and skewness distributions for the Ramp pdf as a function of α'.