Institute of Space and Aeronautical Science, University of Tokyo
Report No. 552, November 1977

An Approximate Method for Prediction of Ignition by Thermal Explosion Theory

By

Tadao TAKENO

Summary: A new method of analysis is developed to predict the critical ignition condition in the thermal explosion theory, which is simple and yet can give the correct dependency of the critical Frank-Kamenetskii parameter δ_c on the activation energy. It is shown that in this method the usual Frank-Kamenetskii approximation corresponds to the special case of large activation energy.

1. INTRODUCTION

The behavior of system with exothermic chemical reaction has been studied by a number of investigators and now the thermal explosion theory is well established [*1*, *2*]. The critical condition for ignition to occur is identified with the one for which a steady-state temperature distribution just ceases to exist. To derive the criticality, it is usual to adopt the Frank-Kamenetskii approximation to the exponential term of Arrhenius rate expression. With this approximation the criticality is specified by the maximum value of a single dimensionless parameter δ (Frank-Kamenetskii parameter). The critical value δ_c depends only on the geometry of system and has been evaluated for the simple shapes of slab, cylinder and sphere, and also for more complicated shapes [*3*]–[*5*]. However, it has long been known that the numerical solution with the exact Arrhenius rate expression gives the value of δ_c which also depends on the activation energy [*6*]. The value of δ_c obtained through the F-K approximation is a limiting value which is accurate only for large values of activation energy. Recently, there are several studies [*7*], [*8*], which aim to obtain the exact values of δ_c by means of numerical solution. Although the method of numerical solution is quite familiar and there are no essential difficulties in obtaining critical values, the numerical integration of two point boundary value problem is rather laborious, especially when the accurate values are wanted. In order to overcome this difficulty, a new method of analysis which can predict the correct dependency of δ_c on activation energy has been developed and the main idea has been described in a brief communication [*9*]. The essential point of the method lies in that the argument of exponential term is expanded about the unknown maximum temperature, instead of about the ambient temperature. This is based on the assertion that the chemical reaction rate in the system is governed mostly by the maximum temperature. The equation and the boundary conditions to be solved are found identical with those of the F-K approximation, yet the derived values of δ_c are much more accurate and show the correct dependency on activation energy as is predicted

by the numerical solution. The purpose of the present paper is to supplement the communication and to give a detailed explanation of the proposed method.

2. Governing Equation and F-K Approximation

The dimensionless steady-state heat conduction equation for a one-dimensional solid with an exothermic zeroth order chemical reaction, and the appropriate boundary conditions, are:

$$\frac{d^2\tau}{d\xi^2}+\frac{j}{\xi}\frac{d\tau}{d\xi}+B\exp\left(-\frac{E_n}{\tau}\right)=0\,, \tag{1}$$

$$\tau'(0)=0\,,\quad \tau(1)=1\,, \tag{2}$$

where $\tau=T/T_0$ is temperature made nondimensional by the ambient temperature T_0, $\xi=x/L$ is the space coordinate made nondimensional by the half-length L of the system, and j is an integer denoting the shape of system. It is equal to 0, 1 and 2 for slab, cylinder and sphere, respectively. The dimensionless parameters B and E_n are defined by

$$B\equiv\frac{AQL^2}{\lambda T_0}\,,\quad E_n\equiv\frac{E}{R^0T_0}\,, \tag{3}$$

where A, Q, λ, E and R^0 are frequency factor, exothermicity, thermal conductivity, activation energy and the universal gas constant, respectively. When we can find a solution for Eqs. (1) and (2) for a given set of values of B and E_n, the heat production rate by chemical reaction just balances the heat loss rate by conduction and the steady state is attained. In this case the ignition will not occur. If we cannot find solutions for another set of values of B and E_n, the steady state cannot be realized since the heat production rate exceeds the heat loss rate and the temperature will increase in time resulting in the spontaneous ignition of system. In the former case, the steady-state temperature is not so high above the ambient temperature, with the nondimensional maximum temperature τ_m close to unity. The nondimensional activation energy E_n is, in general, large as compared to unity. Therefore, we seek a solution in the form

$$\tau(\xi)=1+\frac{1}{E_n}\theta(\xi)+\left(\frac{1}{E_n}\right)^2\theta_1(\xi)+\cdots\,.$$

For simplicity we truncate the series after the second term

$$\tau(\xi)=1+\frac{1}{E_n}\theta(\xi) \tag{4}$$

and the argument of exponential is expanded and approximated as

$$\frac{E_n}{\tau}=E_n-\theta\,. \tag{5}$$

Consequently, the equation and boundary conditions for $\theta(\xi)$ reduce to

$$\frac{d^2\theta}{d\xi^2}+\frac{j}{\xi}\frac{d\theta}{d\xi}+\delta\exp(\theta)=0\,, \tag{6}$$

$$\theta'(0) = \theta(1) = 0\,, \tag{7}$$

where

$$\delta \equiv BE_n \exp(-E_n)\,. \tag{8}$$

The approximation (5) is called as F-K (Frank-Kamenetskii) approximation and the dimensionless parameter δ as F-K parameter. Mathematically, this approximation simplifies the exponential term to enable to obtain the analytical solution. Physically, it elucidates the fact that the ignition process is governed mostly by the single parameter δ, instead of the original two parameters B and E_n.

Equations (6) and (7) indicate that $\theta'(\xi)$ should become negative for $\xi>0$ so long as $\delta>0$. Then $\theta(\xi)$ has only one maximum at $\xi=0$ and the nondimensional maximum temperature τ_m is given by

$$\tau_m = 1 + \frac{1}{E_n}\theta(0)\,, \tag{9}$$

where $\theta(0)$ is to be obtained as an eigenvalue of Eqs. (6) and (7). The latter equations can be solved analytically for $j=0$ and 1, and the parameter δ is related to the eigenvalue $\theta(0)$ by

$$\delta = 2\exp(-\theta(0))\left[\cosh^{-1}\left\{\exp\left(\frac{\theta(0)}{2}\right)\right\}\right]^2 \quad (\delta \geq 0)\,, \tag{10}$$

$$\delta = -2\exp(-\theta(0))\left[\cos^{-1}\left\{\exp\left(\frac{\theta(0)}{2}\right)\right\}\right]^2 \quad (\delta \leq 0) \tag{11}$$

for $j=0$ and

$$\delta = 8\exp(-\theta(0))\left[\exp\left(\frac{\theta(0)}{2}\right) - 1\right] \quad (\delta \leqq 0) \tag{12}$$

for $j=1$. Although in the present analysis these relations have a definite meaning only for $\delta\geq 0$. However, the extension to the region $\delta<0$ will be useful in a future

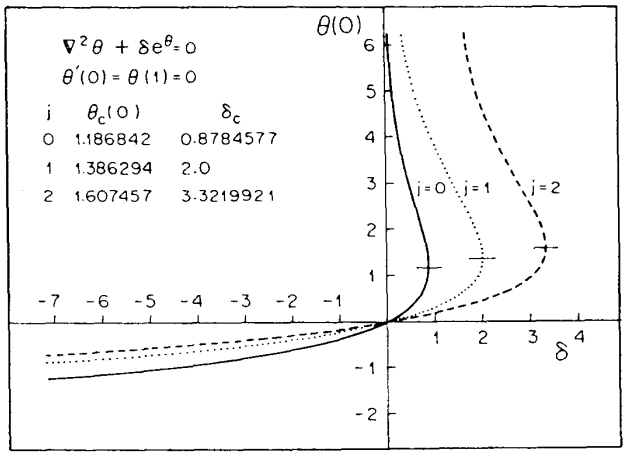

FIG. 1. Relation between Eigenvalue $\theta(0)$ and Parameter δ of Eqs. (6) and (7).

TABLE 1. Eigenvalue $\theta(0)$ as Function of Parameter δ of Eqs. (6) and (7) for Spherical Symmetry ($j=2$).

$-\delta$	$-\theta(0)$	$-\delta$	$-\theta(0)$	δ	$\theta(0)$	$\theta(0)$
0.1	0.01647546	3.1	0.39158011	0.1	0.01686449	
0.2	0.03258100	3.2	0.40138467	0.2	0.03413867	
0.3	0.04833427	3.3	0.41106732	0.3	0.05184501	
0.4	0.06375165	3.4	0.42063124	0.4	0.07000794	
0.5	0.07884837	3.5	0.43007951	0.5	0.08865415	
0.6	0.09363859	3.6	0.43941506	0.6	0.10781285	
0.7	0.10813553	3.7	0.44864073	0.7	0.12751611	
0.8	0.12235155	3.8	0.45775924	0.8	0.14779928	
0.9	0.13629818	3.9	0.46677322	0.9	0.16870146	
1.0	0.14998626	4.0	0.47568518	1.0	0.19026604	
1.1	0.16342597	4.1	0.48449755	1.1	0.21254142	
1.2	0.17662685	4.2	0.49321267	1.2	0.23558179	
1.3	0.18959790	4.3	0.50183280	1.3	0.25944816	
1.4	0.20234760	4.4	0.51036012	1.4	0.28420957	
1.5	0.21488395	4.5	0.51879672	1.5	0.30994464	
1.6	0.22721452	4.6	0.52714464	1.6	0.33674347	
1.7	0.23934645	4.7	0.53540583	1.7	0.36471012	6.04155371
1.8	0.25128652	4.8	0.54358219	1.8	0.39396570	5.40205606
1.9	0.26304114	4.9	0.55167555	1.9	0.42465250	4.99208137
2.0	0.27461641	5.0	0.55968767	2.0	0.45693948	4.66637095
2.1	0.28601811	5.1	0.56762026	2.1	0.49102962	4.38781271
2.2	0.29725176	5.2	0.57547499	2.2	0.52717014	4.13993874
2.3	0.30832257	5.3	0.58325345	2.3	0.56566702	3.91358244
2.4	0.31923554	5.4	0.59095721	2.4	0.60690620	3.70288075
2.5	0.32999542	5.5	0.59858776	2.5	0.65138557	3.50366539
2.6	0.34060675	5.6	0.60614657	2.6	0.69976551	3.31267177
2.7	0.35107385	5.7	0.61363504	2.7	0.75295280	3.12706503
2.8	0.36140087	5.8	0.62105456	2.8	0.81224944	2.94406783
2.9	0.37159175	5.9	0.62840644	2.9	0.87964060	2.76053606
3.0	0.38165029	6.0	0.63569200	3.0	0.95842230	2.57724356
				3.1	1.05483920	2.37218582
				3.2	1.18391066	2.14471316
				3.3	1.41664248	1.81829045

study and hence is included here. The solution for $j=2$ can only be obtained by numerical calculation and Table 1 gives the calculated $\theta(0)$ as the function of δ. Figure 1 shows the relation between $\theta(0)$ and δ and it can be seen that there exists a maximum value of δ above which we have no steady state solutions. The critical value δ_c is a constant depending only on j and found to be 0.87845768, 2.0, 3.32199214 for $j=0$, 1, 2, respectively. The corresponding values of $\theta_c(0)$ are 1.186842, ln 4=1.386294, 1.607457, respectively. The dotted curves in Figs. 2 and 3 show examples of calculated τ_m as the function of δ.

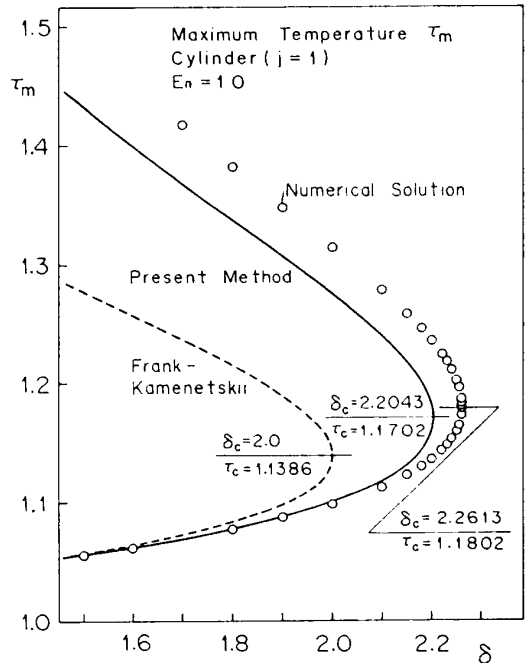

FIG. 2. Maximum Temperature τ_m as Function of δ. Comparison of Three Different Methods.

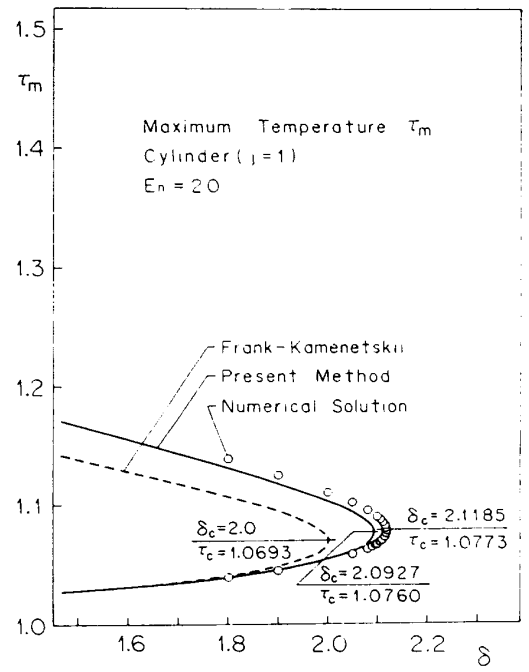

FIG. 3. Maximum Temperature τ_m as Function of δ. Comparison of Three Different Methods.

3. Method based on Expansion about Maximum Temperature

In the F-K approximation, the temperature is expanded about the ambient temperature and the approximation is exact at $\tau=1$, while it is worst at $\tau=\tau_m$. This is unfavorable since the reaction rate is governed mainly by the maximum temperature. It is better to adopt the method of expansion which is most accurate at $\tau=\tau_m$. This can be done by introducing a new dependent variable $\varphi(\xi)$,

$$\tau(\xi) = \tau_m - \frac{\tau_m^2}{E_n}\varphi(\xi)\,. \tag{13}$$

Then the argument of the exponential term is expanded and approximated as

$$\frac{E_n}{\tau} = \frac{E_n}{\tau_m} + \varphi\,. \tag{14}$$

The equation and boundary conditions for $\varphi(\xi)$ reduce to

$$\frac{d^2\varphi}{d\xi^2} + \frac{j}{\xi}\frac{d\varphi}{d\xi} - \varepsilon \exp(-\varphi) = 0\,, \tag{15}$$

$$\varphi'(0) = 0\,, \quad \varphi(1) = b\,, \tag{16}$$

where

$$\varepsilon \equiv \frac{BE_n}{\tau_m^2}\exp\left(-\frac{E_n}{\tau_m}\right), \tag{17}$$

$$b \equiv \frac{(\tau_m - 1)}{\tau_m^2}E_n\,. \tag{18}$$

Since τ is maximum at $\xi=0$, there is another condition

$$\varphi(0) = 0 . \tag{19}$$

Now we have three boundary conditions for the second order equation. One extra condition makes it possible to determine the unknown quantity b, and hence the unknown maximum temperature τ_m, as the eigenvalue of the equations. The method of solution is straightforward. For a given value of E_n and an arbitrary value of ε, Eq. (15) with the boundary conditions (19) and the first part of (16) is solved as an initial value problem, and the value of b can be determined. This in turn makes it possible to calculate τ_m by using Eq. (18) as

$$\tau_m = \frac{E_n}{2b}\left\{1 \pm \left(1-\frac{4b}{E_n}\right)^{1/2}\right\} . \tag{20}$$

Substitution of the calculated τ_m into Eq. (17) yields the value of B and hence of δ for the prescribed value of ε. The calculation is repeated for other values of ε and we obtain τ_m as a function of δ for the given E_n. In Eq. (20) the upper plus sign corresponds to $\tau_m \geq 2$, while the lower minus sign corresponds to $2 \geq \tau_m \geq 1$. In the present analysis of ignition, we are concerned with τ_m close to unity and hence only the minus sign will be considered hereafter.

The above described method seems to require the solution of the new Eq. (15). However, this can be avoided as follows. We introduce another dependent variable $\psi(\xi)$,

$$\psi(\xi) = b - \varphi(\xi) . \tag{21}$$

Then the equation and boundary conditions for $\psi(\xi)$ reduce to*

$$\frac{d^2\psi}{d\xi^2} + \frac{j}{\xi}\frac{d\psi}{d\xi} + \Delta \exp(\psi) = 0 , \tag{22}$$

$$\psi'(0) = \psi(1) = 0 , \quad \psi(0) = b , \tag{23}$$

where

$$\Delta \equiv \frac{\delta}{\tau_m^2} \exp\left\{E_n\left(\frac{\tau_m - 1}{\tau_m}\right)^2\right\} . \tag{24}$$

Now we find the derived Eqs. (22) and (23) are identical with Eqs. (6) and (7) of the F-K approximation. Moreover, we notice that the quantity b defined by Eq. (18) is just the eigenvalue of the equations. Therefore, the relation between the eigenvalue b and the parameter Δ is exactly the same as that between $\theta(0)$ and δ of the F-K approximation. We can utilize the relations given by Eqs. (10) through (12) and by Table 1, by replacing $\theta(0)$ by b and δ by Δ. Now the method of calculation is very simple. For a given value of E_n and an arbitrary value of τ_m, we calculate b by using

* When Eqs. (21) and (18) are substituted into Eq. (13), $\tau = 1 + \tau_m^2 \psi / E_n$ is obtained. If this expression is further substituted into Eq. (1), the resulting equation does not coincide with Eq. (22). This is because in the process of derivation the argument of exponential is expanded about unity and not about τ_m as in the case of Eq. (22).

Eq. (18) and then the value of Δ can be determined. Substitution of the latter into Eq. (24) yields the value of δ. Thus we obtain τ_m as a function of δ for the given E_n. The solid curves in Figs. 2 and 3 show examples of the calculated τ_m as the function of δ, as compared to the dotted curves of the F-K approximation and also to open circles of the exact numerical solution. The latter has been obtained by solving numerically the original boundary value problem of Eqs. (1) and (2). It can be seen that the present analytical method gives the solution which is very close to the exact solution and brings about a significant improvement in the accuracy. In these figures the critical values τ_c and δ_c, derived by the respective method, are also shown. The present method predicts the larger critical values than the F-K approximation, but they are still smaller than the exact values. The accuracy of the derived critical values increase with the increase of E_n.

4. Correlation of Present Method with F-K Approximation

Although it is now possible by means of the present method to calculate τ_m as the function of δ for any given value of E_n, it will be instructive to examine its correlation with the F-K approximation. The two methods utilize the identical relation between the eigenvalue b and the parameter Δ of Eqs. (22) and (23), yet the derived values of τ_m and δ are different for the two methods because of the following two causes. Firstly, for a given value of b the present method calculate τ_m through Eq. (20), while the F-K approximation uses Eq. (9), in which $\theta(0)$ should be replaced by b. Figure 4 compares the derived τ_m as the function of b/E_n. In Eq. (20) E_n is large as compared to unity, while b is the order of unity as is seen in Fig. 1. Then the expansion of the root for small values of b/E_n gives

$$\tau_m = 1 + \frac{b}{E_n} + 2\left(\frac{b}{E_n}\right)^2 + \cdots \tag{25}$$

which reveals that τ_m of the F-K approximation corresponds to the first two terms of the present method. Secondly, in view of Eq. (24) we have

$$\delta = G\Delta \tag{26}$$

where

$$G \equiv \tau_m^2 \exp\left\{-E_n\left(\frac{\tau_m - 1}{\tau_m}\right)^2\right\}. \tag{27}$$

Therefore, in the present method Δ must be multiplied by the factor G in order to obtain δ, whereas in the F-K approximation Δ is just equal to δ. For a fixed value of E_n, G is a function of τ_m or if Eq. (20) is used it is a function of b. Figure 5 represents G as the function of b with E_n as a parameter. G becomes maximum at $b=1$ and the maximum value decreases with the decrease of $1/E_n$. When Eq. (27) is expanded for small values of $1/E_n$ for a fixed value of b, we have

$$G = 1 + \frac{b}{E_n}(2 - b) + \cdots \tag{28}$$

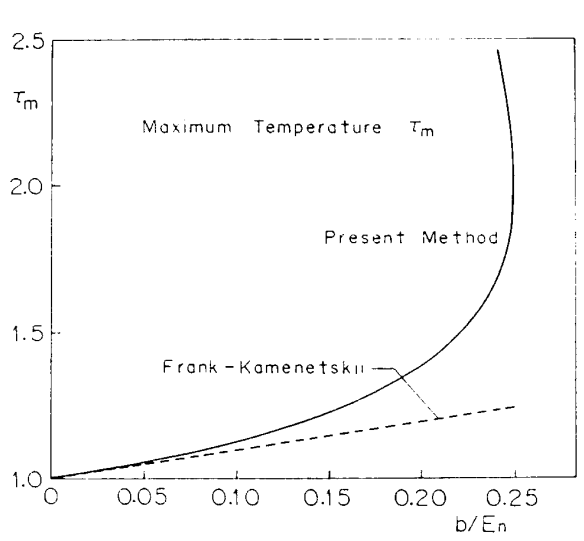

FIG. 4. Maximum Temperature τ_m as Function of b/E_n. Comparison of Two Approximate Methods.

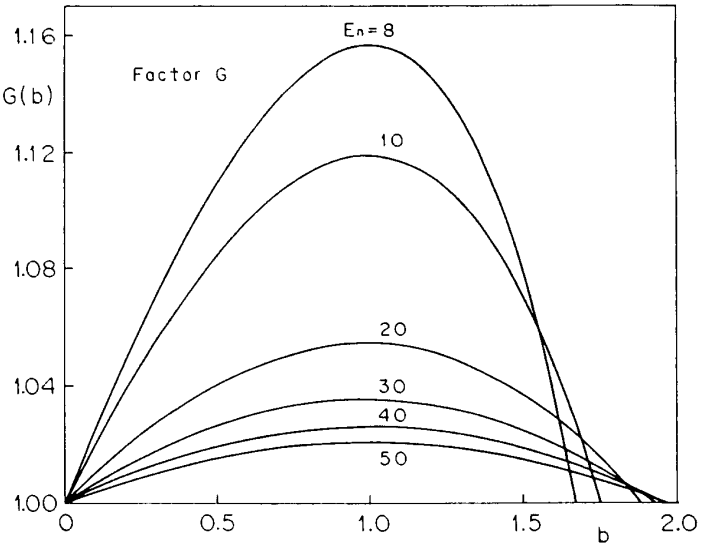

FIG. 5. Factor G as Function of b with E_n as Parameter.

which indicates that in the limit of small $1/E_n$, Δ becomes equal to δ. It is interesting to note that in the F-K approximation τ_m is valid to the first order of $1/E_n$, whereas δ cannot account for the effect of E_n at all. In any way we see that in the present method the F-K approximation corresponds to the special case of large activation energy.

5. CRITICALITY

In the present method the critical values τ_c and δ_c can be determined analytically. For a fixed value of E_n, the independent variable is τ_m or b and the criticality is given by

$$\frac{d\delta}{d\tau_m} = \frac{d\delta}{db}\frac{db}{d\tau_m} = 0 . \tag{29}$$

Differentiation of Eq. (26) yields

$$\frac{1}{\delta}\frac{d\delta}{db} = \frac{1}{\Delta}\frac{d\Delta}{db} + \frac{1}{G}\frac{dG}{db} , \tag{30}$$

while that of Eqs. (20) and (27) yields

$$\frac{1}{G}\frac{dG}{db} = \frac{1}{G}\frac{dG}{d\tau_m}\frac{d\tau_m}{db} = \frac{(b-1)}{b} - \frac{(b-1)}{b}\left(1 - \frac{4b}{E_n}\right)^{-1/2} . \tag{31}$$

Substitution of Eqs. (30) and (31) into Eq. (29) yields

$$\frac{d\delta}{d\tau_m} = \delta\left(\frac{db}{d\tau_m}\right)\left[\frac{d}{db}(\ln \Delta) + \frac{(b-1)}{b} - \frac{(b-1)}{b}\left(1 - \frac{4b}{E_n}\right)^{-1/2}\right] . \tag{32}$$

On the other hand, from Eq. (18) we obtain

$$\frac{db}{d\tau_m} = \frac{E_n}{\tau_m^3}(2 - \tau_m) , \tag{33}$$

which indicates that $(db/d\tau_m)>0$ for $1<\tau_m<2$. In view of $\delta>0$, the criticality is now reduced to

$$\frac{(b-1)}{(b-1)+b(d(\ln \Delta)/db)}=\left(1-\frac{4b}{E_n}\right)^{1/2}. \tag{34}$$

This is the equation to be used to determine the critical values b_c and Δ_c, when Δ is given as a function of b. The left-hand side is the function of b only, while the right-hand side contains the parameter E_n. By plotting the left-hand side against b, and then the right-hand side for a given value of E_n, we can determine the critical value b_c for that value of E_n from the cross point of the two curves. Then the critical value Δ_c can be determined. Substitution of b_c into Eq. (20) yields τ_c, and then δ_c is obtained through Eqs. (26) and (27). The examination of Eq. (34) reveals that the limiting value of $b_c=1$ is obtained for $E_n=4$ on one hand, and of $b_c=\theta_c(0)$ for $E_n\to\infty$ on the other hand. In the latter case, δ_c coincides with that of the F-K approximation.

When Eqs. (10) and (12) are substituted into the left-hand side of Eq. (34), which is now denoted here as $F(b)$, we have

$$F(b)=\frac{(b-1)\{1-\exp(-b)\}^{1/2}\cosh^{-1}\{\exp(b/2)\}}{b-\{1-\exp(-b)\}^{1/2}\cosh^{-1}\{\exp(b/2)\}} \tag{35}$$

for $j=0$, and

$$F(b)=\frac{2(b-1)\{\exp(b)-1\}}{(b-2)\exp(b/2)+2} \tag{36}$$

for $j=1$, respectively. For $j=2$, we have to resort to numerical calculation. As an example of the determination of the critical value b_c, the case for $j=1$ is shown in Fig. 6. It can be seen that b_c is restricted in the range $1\leq b_c\leq \ln 4$ for the variation

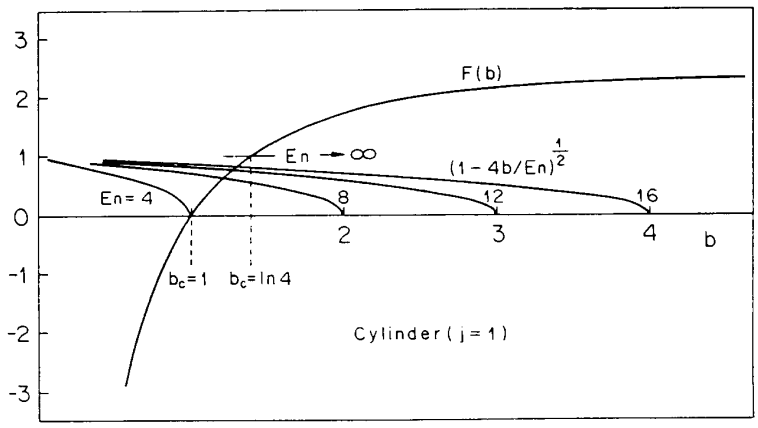

FIG. 6. Determination of Critical Value b_c by Means of Eq. (34).

of E_n between 4 and infinity. Figure 7 compares the critical maximum temperature τ_c calculated by the three methods. The numerical solution is obtained from the paper by Shouman et al. [7]. It can be seen that the prediction by the present method correlates satisfactory with the exact solution. Figure 8 compares the critical F-K parameter δ_c obtained by the present method with that of the numerical solution [6], [7].

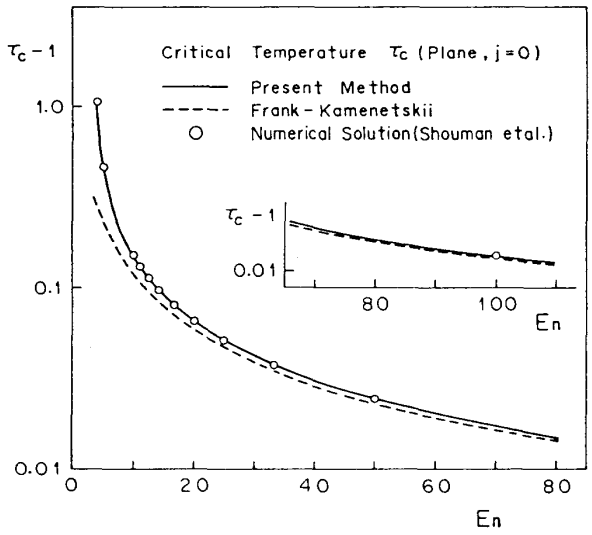

FIG. 7. Critical Maximum Temperature τ_c as Function of E_n. Comparison of Three Different Methods.

As was pointed out before, the F-K approximation cannot account for the effect of E_n on δ_c but only gives the limiting value of large E_n. On the other hand, we see that the present analytical method can predict the correct dependency of δ_c on E_n as is predicted by the exact numerical solution. The effect of E_n becomes more important with the increase of j, while the accuracy of the prediction increases, as is expected, with E_n and decreases with the increase of j. Figure 9 compares the accuracy of the critical values predicted by the two analytical methods, on the basis of the exact numerical solution [7]. We see here again that the present method has brought about an significant improvement. These results shown in Figs. 7 through 9 indicate that the accuracy of the proposed method is satisfactory over a wide range of E_n and it is almost unnecessary to solve numerically the original two point boundary value problem.

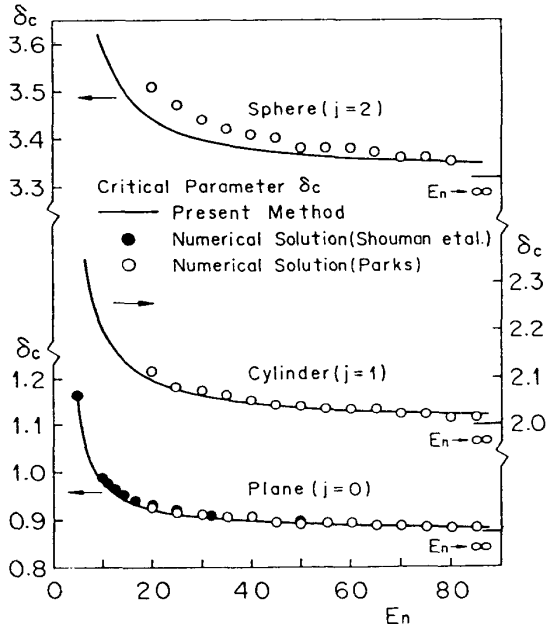

FIG. 8. Critical F-K Parameter δ_c as Function of E_n. Comparison between Present Method and Numerical Solution.

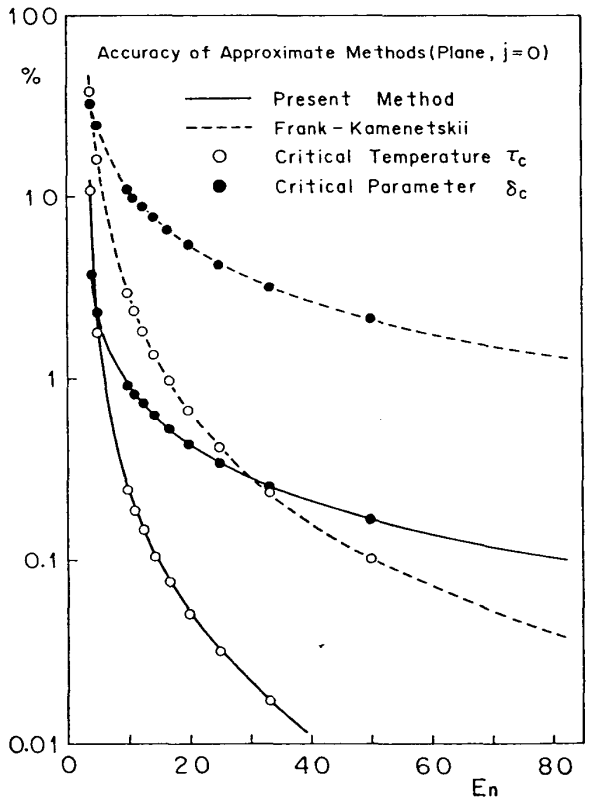

FIG. 9. Accuracy of two Approximate Analytical Methods for Critical Values τ_c and δ_c.

6. Discussions

The excellent correlation between the present method and the exact numerical solution confirms the validity of the premise, on which it is based, that the chemical reaction rate in the system is mostly governed by the maximum temperature. The predicted critical values, as well as those of the F-K approximation, are always larger than those of the numerical solution. This is because the present method of expansion about the maximum temperature still overestimates the chemical reaction rate. The expansion (14) is valid only to the first order of the small quantity $\tau_m\varphi(\xi)/E_n$. Since the maximum value of $\varphi(\xi)$ is given by b, when Eq. (18) is used we find that the accuracy depends on $(\tau_m-1)/\tau_m$. Therefore, the application of this method may not be restricted to the spontaneous ignition problem, so long as the critical value of this quantity remains small. Moreover, the method concerns only the expansion of the exponential term and is independent of the form and boundary conditions of governing equations. Although in the present paper the method was applied for the simple one-dimensional geometry and symmetric boundary conditions, it can be applied for any other shapes and boundary conditions. The only restriction is that there should be one maximum temperature in the field. Therefore, it may also be applied for other problems of combustion phenomena, in which the nonlinear effect of Arrhenius rate expression plays a crucial role.

The author gratefully acknowledges the assistance of Mr. Y. Kotani and Mr. K. Sato with the numerical calculation.

Department of Jet Propulsion
Institute of Space and Aeronautical Science
University of Tokyo
September 28, 1977

References

[1] Akita, K.: Combustion Research *9* (in Japanese), 2–40 (1965).
[2] Gray, P. and Lee, P. R.: in Oxidation and Combustion Reviews (C. F. H. Tipper, Ed.), Elsevier, Amsterdam, London, New York, 1967, Vol. 2, p. 1.
[3] Boddington, T., Gray, P. and Harvey, D. I.: Combust. Flame *17*, 263–265 (1971).
[4] Boddington, T., Gray, P. and Harvey, D. I.: Phil. Trans. Roy. Soc., *270*, 467–506 (1971).
[5] Boddington, T., Gray, P., Griffiths, J. F. and Hart, A. D.: 2nd European Symp. on Combustion, Combustion Inst., Pittsburgh, 1975, p. 539.
[6] Parks, J. R.: J. Chem. Phys. *34*, 46–50 (1961).
[7] Shouman, A. R., Donaldson, A. B. and Tsao, H. Y.: Combust. Flame *23*, 17–28 (1974).
[8] Shouman, A. R. and Donaldson, A. B.: Combust. Flame *24*, 203–210 (1975).
[9] Takeno, T.: Combust. Flame *29*, 209–211 (1977).