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by

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ABSTRACT

A computational procedure is described for determining the thermal conductivity of a material from experimentally determined transient cooling data.

INTRODUCTION

In this report, we describe a procedure that we have developed to determine the thermal conductivity of graphite. The method can be divided into two distinct parts. First, the transient cooling profile of a cylindrical sample of the material is experimentally determined. These data have been provided by Paul Wagner.[1] Second, we simulate this cooling on the CDC 6600 computer by solving a set of finite difference equations. We will describe this numerical simulation, and indicate how this process can be used to approximate the thermal conductivity of the material.

The procedure has been successfully applied to a test case which is a model of the graphite experimental data. An essential feature of the method is that it automatically indicates whether the experimental data are accurate enough for the computational results to be meaningful. No solution is obtained when the procedure is applied to the graphite laboratory data, and we feel that this is due both to inaccuracies in the experimental data and to the fact that the computational model does not adequately describe the laboratory experiment. Nevertheless, the results for the test case indicate that this method could be very useful in similar problems with more accurate input data.

FORMULATION OF THE PROBLEM

In the laboratory procedure, the ends of a cylindrical sample of a material are heated to a temperature at which the heat flow has reached a steady state. The heating is then stopped, and the cooling profile as a function of time at several points in a radial direction is observed. We assume that the length-to-radius ratio of the sample is large enough to justify neglecting the end effects, and also that the material is homogeneous.

Under these conditions, the temperature $T = T(t, r)$ satisfies the nonlinear initial value problem,

$$\left.\begin{aligned} \frac{\partial T}{\partial t} &= \frac{1}{r}\frac{\partial}{\partial r}\left(r\alpha(T)\frac{\partial T}{\partial r}\right) \qquad (0 < r < R_1,\ t > 0) \\ T(0, r) &= g(r) \qquad (0 \le r \le R_1) \end{aligned}\right\}, \tag{1}$$

and the two sets of boundary conditions,

$$\left.\begin{aligned} \frac{\partial T}{\partial r}(t, 0) &= 0 \qquad (t > 0) \\ T(t, R_1) &= f_1(t) \qquad (t > 0) \end{aligned}\right\} \tag{2}$$

and

$$T(t, 0) = f_0(t) \qquad (t > 0)\ . \tag{3}$$

The notation used in these equations is the following:

(i) R is the radius of the cylindrical sample, and $0 < R_1 < R$.

(ii) The thermal diffusivity, $\alpha(T)$, is given by

$$\alpha(T) = \frac{k(T)}{\rho(T)\, C_p(T)} \quad .$$

The thermal conductivity, $k(T)$, is assumed to have the form

$$k(T) = \frac{A}{T} + B \quad ,$$

and the unknown nonnegative constants A and B are to be determined by the computational procedure. The density, $\rho(T)$, is given by

$$\rho(T) = \frac{\rho_0}{1 + \rho_1 (T - \rho_2)} \quad ,$$

and the constants ρ_i are known. The specific heat, $C_p(T)$, is assumed to be known, although only in tabular form.

(iii) The boundary condition $\frac{\partial T}{\partial r}(t, 0) = 0$ is satisfied because $T(t, r)$ is "symmetric" about $r = 0$.

(iv) The functions $f_0(t)$ and $f_1(t)$ for the boundary conditions at $r = 0$ and $r = R_1$ are assumed to be known from the experimental data.

(v) Because the material is at a steady state at $t = 0$, we assume that the function $g(r)$ in the initial condition is the parabola given by

$$g(r) = f_0(0) + \left(f_1(0) - f_0(0)\right)\left(\frac{r}{R_1}\right)^2 \quad .$$

We have selected the boundary conditions in Eqs. (2) and (3) with $R_1 < R$ for our computational model for two reasons. First, the choice of Dirichlet data for $T(t, r)$ on the line $r = \text{constant} > 0$ simplifies the mathematical model because we do not have to consider a radiation boundary condition at the surface of the cylinder. Second, we believe that the experimental data from the interior of the cylinder ($r = R_1$) are more reliable than data from the surface of the cylinder ($r = R$).

We now consider the initial-boundary value problem (P) defined by Eq. (1) with the boundary conditions in Eq. (2). We assume that for each fixed A and B there is a unique solution $T(t, r)$ to problem (P). This is a reasonable hypothesis on physical grounds, but we do not know enough about the function $\alpha(T)$ to prove that this assumption is always satisfied. For a given A and B, it is clear that the solution $T(t, r)$ to problem (P) will not generally also satisfy Eq. (3). Because the solution derived in the laboratory does satisfy both equations, we see that this yields an overdetermined problem. The goal of the computational procedure is to determine values of A and B such that the solution to problem (P) also satisfies Eq. (3). On physical grounds, we expect a unique solution pair (A, B) to exist.

There is an extensive literature dealing with overdetermined problems similar to the one we are considering. In particular, we cite the work of Cannon,[2-5] Cannon, Douglas, and Jones,[6] Cannon and Halton,[7] Cannon and Jones,[8] Douglas and Jones,[9] and Jones.[10,11] In general, these authors restrict their attention to the linear case in which the thermal diffusivity depends only on the time t, and their results do not seem to be directly applicable to our problem.

In two recent papers Cannon, DuChateau, and Filmer[12,13] have described a method that we have incorporated in our procedure. We are grateful to Prof. J. R. Cannon[14] for discussing this technique with us and indicating how it could be applied to our particular overdetermined problem.

THE COMPUTATIONAL PROCEDURE

Let t_1^*, t_2^*, and t_3^* be three fixed times satisfying

$$0 < t_1^* < t_2^* < t_3^* \le \tau \quad ,$$

where τ is the maximum time considered. Let $T(t, r; A, B)$ be a solution to problem (P), and fix t^* at one of the values t_i^*. For each value of A in a prescribed interval, we try to find a value for $B = B(A)$ such that

$$T\left(t^*, 0; A, B(A)\right) = f_0(t^*) \quad .$$

This defines a curve $\left(A, B(A)\right)$ for each value of t^*, and we then find the points of intersection of the three curves corresponding to t_1^*, t_2^*, and t_3^*. If the points of intersection are (A_i, B_i)

for $1 \le i \le 3$, we define the approximate solution pair (A, B) by

$$A = \frac{1}{3}(A_1 + A_2 + A_3) \quad ,$$

$$B = \frac{1}{3}(B_1 + B_2 + B_3) \quad .$$

We are not able to guarantee a priori that this method will provide a solution to the problem. This question is discussed by Cannon, DuChateau, and Filmer,[12] but we cannot show that the hypotheses of their theorem are satisfied. Nevertheless, our computational results provide experimental justification for the application of the method to this particular problem.

In Appendix A we have outlined another procedure that we have used for this problem. It is more time-consuming and much less accurate than the method described above, so no numerical results are included.

COMPUTATIONAL RESULTS

We have used the computational procedure outlined in the preceding section on two different problems. The first example is a test problem that was selected to determine the feasibility and accuracy of the method. The second problem is derived from the laboratory data for graphite.

For the test problem, we let $\rho_0 = 1.75$, $\rho_1 = 1.5 \times 10^{-5}$, $\rho_2 = 300$, $R_1 = 0.635$, and we let $C_p(T)$ be determined by the values given in Ref. 1. Define

$$f_1(t) = 2463\, e^{-0.04t} \quad ,$$

$$A = 530 \quad ,$$

$$B = 0.18 \quad ,$$

which are the approximate values for graphite. Solve problem (P) with these values and $f_0(0) = 2512$, and call the solution $T_0(t, r)$. We then let $f_0(t) = T_0(t, 0)$, and use this function as input to the computer program. The solution to problem (P) is approximated by the solution to a finite difference equation, and this process is described in Appendix B.

In Figs. 1 to 4 we have plotted the computational results for the test case with a varying number of correct digits for the input data $f_0(t)$. The three curves in each case are for $t_1^* = 4$, $t_2^* = 9$, and $t_3^* = \tau = 14$. Note that the method works very well with accurate input data, but its usefulness rapidly deteriorates as the number of correct digits in $f_0(t)$ is decreased. The data for the graphs in Fig. 4 have been perturbed by random noise so that the relative error is less than 0.1%, and our method does not yield a solution.

In Fig. 5 we have plotted the curves for the graphite experimental data. The parameters are the same as those in the test case, except that we use $t_1^* = 4$, $t_2^* = 7$, and $t_3^* = \tau = 9$. In addition, $f_0(t)$ and $f_1(t)$ are determined from the data in Ref. 1. Since the curves in Ref. 1 are for graphite, we would expect to compute $A = 530$ and $B = 0.18$. However, it is clear that the method has not determined a solution, and the computed points on the curves are far from the expected values. In Table I

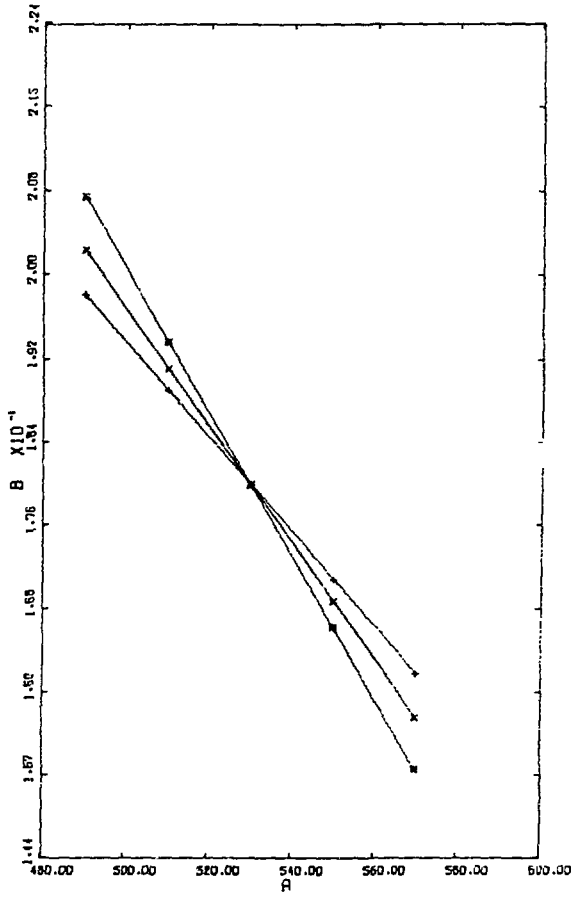

Fig. 1. Test case with ten correct digits in boundary data.

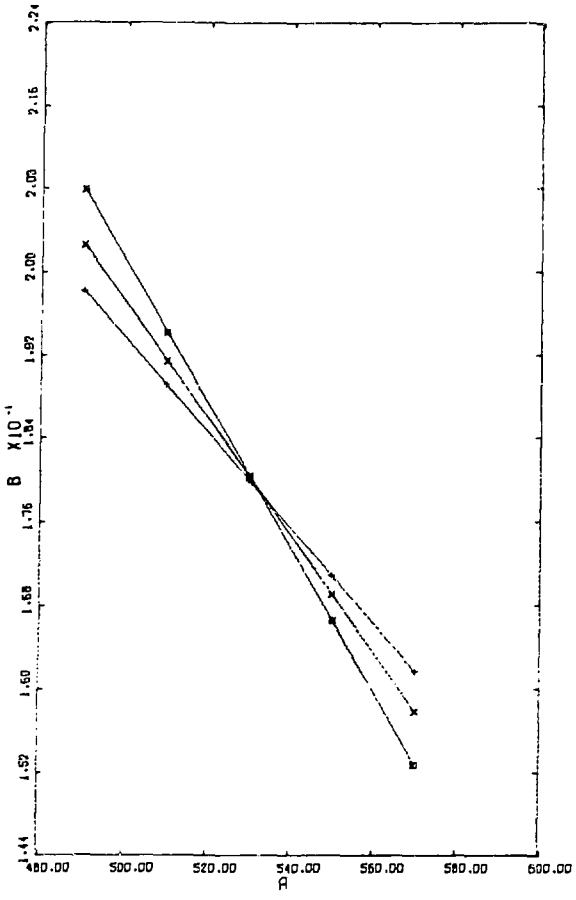

Fig. 2. Test case with five correct digits in boundary data.

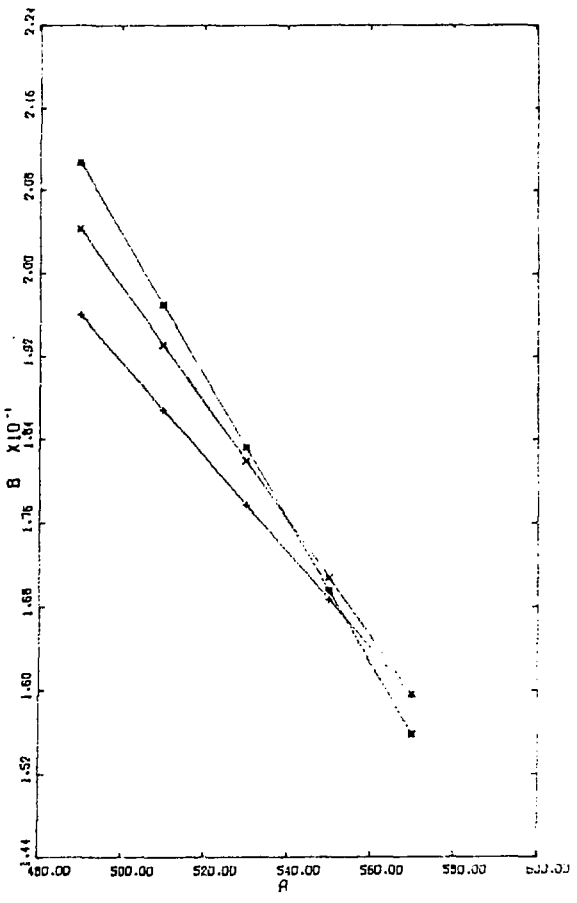

Fig. 3. Test case with four correct digits in boundary data.

we have tabulated the experimentally determined values for $f_0(t)$, which can be compared with the computationally determined values for $f_0(t)$ using $A = 530$, $B = 0.18$, and the experimental data for $f_1(t)$.

CONCLUSIONS

We conclude from these computational results that the method can be applied to overdetermined problems of this form. However, the procedure does not give acceptable results for the graphite experimental data. We feel that this is due to a failure in the model rather than in our method of solution, for the following reasons:

(A) The experimental data may be too inaccurate for the method to yield a solution. As the results for the test case demonstrate, one of the primary advantages of this procedure is that it automatically indicates whether the input data are accurate enough to provide reliable solutions. The graphite curves in Fig. 5 clearly show that this accuracy condition on the input data is not satisfied.

(B) We may be using the wrong model for the laboratory experiment. We do not believe that the large discrepancies exhibited in Table I can be accounted for simply as noise in the data. Rather, we feel that the initial-boundary value problem for this partial differential equation does not adequately describe the experiment. The following factors provide a possible explanation:

(1) The sample is too short relative to the radius to justify ignoring the end effects.

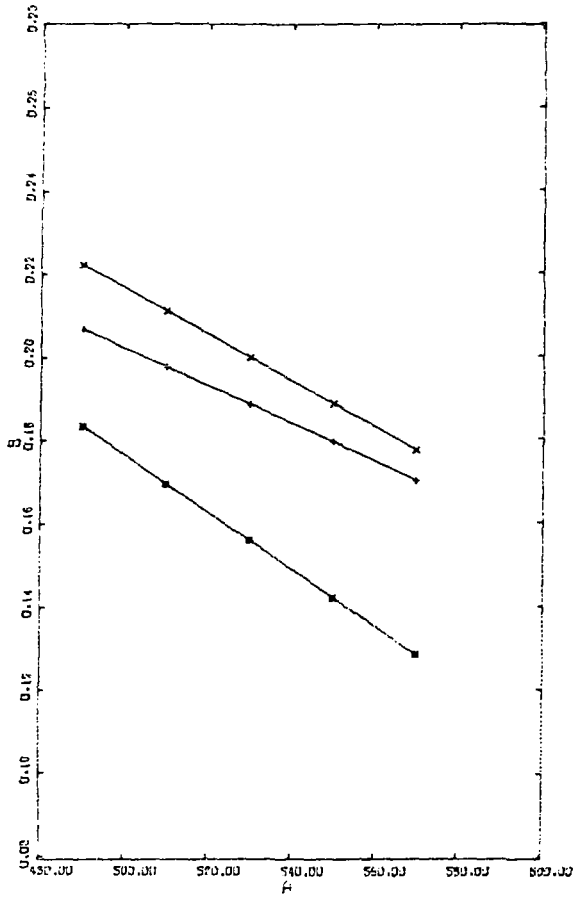

Fig. 4. Test case with three correct digits in boundary data.

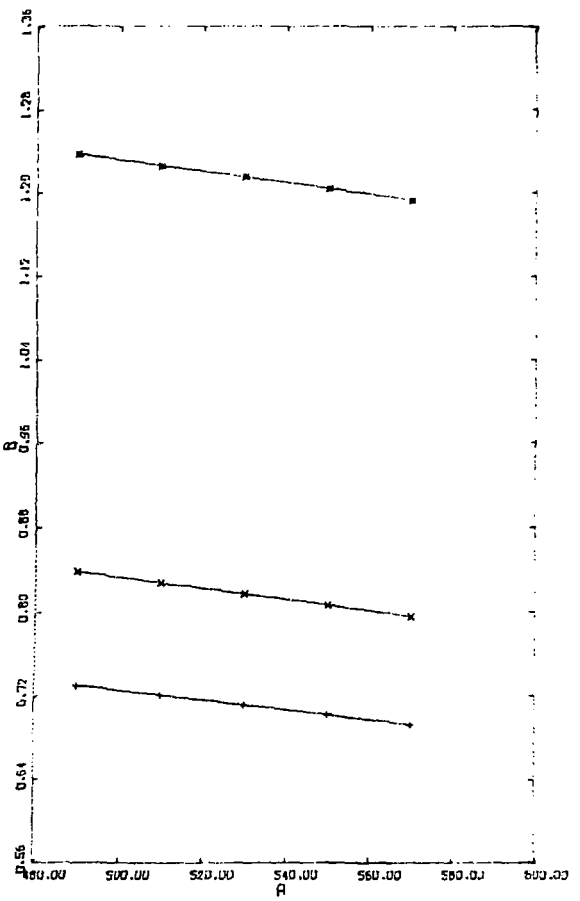

Fig. 5. Graphite experimental data.

(2) The heat flow is not independent of the angular direction.

(3) The sample is not homogeneous.

(4) The data provided are not precisely at $r = 0$, so the boundary condition $\frac{\partial T}{\partial r}(t, 0) = 0$ cannot be used.

(5) The sample is not at a steady state at time $t = 0$.

(6) The approximation of $T(0, r)$ by a parabola is not accurate enough.

(7) The assumed form for $\alpha(T)$ is not adequate to describe the thermal diffusivity for this material under these conditions.

(C) It is possible that we have not solved the finite difference equations accurately enough. In this respect, we have considered the following factors:

(1) The truncation error may be too large because the mesh is too coarse. We have run test cases using Bessel functions, and the mesh size does not appear to be a source of significant error.

(2) We may not be solving the equations accurately enough because of the nonlinearity in $\alpha(T)$. We have used an iterative technique to improve the accuracy of the solutions to the nonlinear problem, and the relative change in temperature is less than 10^{-5}. This would not be a large enough error to account for the graphite results.

(3) The finite difference equations may not have a unique solution pair (A, B). We know

TABLE I

EXPERIMENTAL AND COMPUTED VALUES FOR $f_0(t)$ FOR GRAPHITE DATA WITH $A = 530$ AND $B = 0.18$.

t	Experimental Value	Computed Value
1	2455	2461.26
2	2350	2389.00
3	2247	2293.81
4	2194	2198.30
5	2070	2116.02
6	2001	2041.16
7	1934	1966.63
8	1874	1904.13
9	1823	1850.27

of no results in this direction, and we have been unable to determine whether this is a significant factor in our computational results.

APPENDIX A

ANOTHER METHOD FOR THE SOLUTION OF THE OVERDETERMINED PROBLEM

Let $t_0, t_1, \ldots, t_N$ be a fixed set of points satisfying

$$0 = t_0 < t_1 < t_2 < \ldots < t_N \leq \tau \quad .$$

If $w(t)$ is any given function, the norm $\eta(w)$ is defined by

$$\eta(w) = \left[\sum_{i=1}^{N} w(t_i)^2 \right]^{1/2} \quad .$$

We remark that there are many other norms that could be used for $\eta(w)$, such as $\max_{1 \leq i \leq N} |w(t_i)|$. However, our computational experience indicates that the choice of norm is not critical to the procedure.

If $T(t, r; A, B)$ is a solution to problem (P), we define the error $E(A, B)$ in this function by

$$E(A, B) = \eta\left(T(t, 0; A, B) - f_0(t)\right) \quad .$$

Our goal is to determine values A_0 and B_0 such that

$$E(A_0, B_0) = \min_{A \geq 0, B \geq 0} E(A, B) \quad .$$

Notice that this method of solution uses all of the data on the line $r = 0$, rather than just data at the three points $(t_i^*, 0)$, $1 \leq i \leq 3$. In our computations, we have solved the minimization problem in the form

$$E(A_0, B_0) = \min_{A} \left[\min_{B} E(A, B) \right] \quad .$$

The advantage of this procedure is that the curves $\{E(A, B) | A \text{ fixed}\}$ have always been convex, so the one-dimensional minimization problems are easy to solve.

We have not used this approach for our computational procedure for two reasons. First, it is very time-consuming to evaluate the function $E(A, B)$ (about 4 sec on a CDC 6600 computer), and $E(A, B)$ is steep in the neighborhood of $B = B_0$. This makes the calculation of the function $M(A) \equiv \min_{B} E(A, B)$ quite expensive. Second, the graph of $M(A)$ is very flat near the minimum, and it is not possible to meaningfully ascertain the value of A_0.

APPENDIX B

FINITE DIFFERENCE EQUATIONS

Consider the nonlinear initial-boundary value problem

$$\left.\begin{aligned}
&\frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \alpha(T) \frac{\partial T}{\partial r} \right) && (0 < r < R_1, t > 0) \\
&T(0, r) = g(r) && (0 \leq r \leq R_1) \\
&\frac{\partial T}{\partial r}(t, 0) = 0 && (t > 0) \\
&T(t, R_1) = f_1(t) && (t > 0)
\end{aligned}\right\} .$$

In this appendix, we outline the finite difference approximation we have used for this problem. These techniques are not new, and we refer to Ref. 15 for a complete discussion of similar methods.

Define mesh points (t_i, r_j) by

$$t_i = i \Delta t, \quad \Delta t = \frac{\tau}{N} \quad ,$$

$$r_j = j \Delta r, \quad \Delta r = \frac{R_1}{M} \quad ,$$

and use the notation $T_{ij} = T(t_i, r_j)$. We introduce the difference operator $D_{\alpha_i} T_{ij}$ defined by

$$r_j > 0: \; D_{\alpha_i} T_{ij} = \frac{1}{r_j (\Delta r)^2} \left[(\alpha r)_{i,j-1/2} T_{i,j-1} - \left((\alpha r)_{i,j-1/2} + (\alpha r)_{i,j+1/2} \right) T_{ij} + (\alpha r)_{i,j+1/2} T_{i,j+1} \right] ,$$

$$r_j = 0: \; D_{\alpha_i} T_{ij} = \frac{4\alpha(T_{i0})}{(\Delta r)^2} \left[T_{i1} - T_{i0} \right] ,$$

where

$$(\alpha r)_{i,j+1/2} = \left[\frac{r_j + r_{j+1}}{2} \right] \left[\frac{\alpha(T_{ij}) + \alpha(T_{i,j+1})}{2} \right] .$$

The difference equations we use are given in the implicit form

$$\frac{T_{i+1,j} - T_{ij}}{\Delta t} = D_{\alpha_i} T_{i+1,j}$$

$$(0 \le i \le N - 1 , \; 0 \le j \le M - 1) .$$

For a fully implicit equation, we would use the operator $D_{\alpha_{i+1}} T_{i+1,j}$ in the right-hand side of the equation. However, this choice makes the computation of $T_{i+1,j}$ more difficult, and because $\alpha(T)$ is observed to be a slowly varying function of time it appears that no significant error is introduced by computing the solution by the above "semi-implicit" equation.

We have used the values N = 16 and M = 20 for our numerical results. The function $f_1(t)$ is given by a cubic spline interpolant through the data points $f_1(t_i)$, and we actually compute the solution $T(t, r)$ with $\Delta t = \frac{T}{465}$.

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