OPTIMUM AVERAGE DIFFUSION COEFFICIENT: AN OBJECTIVE INDEX IN DESCRIPTION OF WOOD DRYING DATA[1]

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ABSTRACT

In the existing schemes for estimating average diffusion coefficients, the equations are approximate because of the use of only the first term in an infinite series and the subjective nature of the methods. The method described here takes into account all data points, and provides a systematic and objective way of analyzing wood drying data. Using the formula of the theoretical Fourier series solution, a series of theoretical $\bar{E}$ values, representing the fractional amounts of water in wood during drying, were coupled with experimental data, and the sum of squares minimized. The method sets up upper and lower expected bounds for diffusion coefficients, and then locates the optimum average diffusion coefficient by using a FORTRAN program based on the *golden section search* principle. Using data from a previous drying study on six hardwoods, it was found that the theoretical curves in the longitudinal direction fitted the data points satisfactorily. This suggests that diffusion coefficients in the longitudinal direction are virtually constant. This method, however, depends upon the assumption that the value of $\bar{E}$ at the surface drops immediately to zero as drying starts.

Keywords: Drying, diffusion-coefficient, optimization, Fourier series, golden section search.

INTRODUCTION

The moisture diffusion coefficient is an important index in determining the drying rate of wood. Although the surface emission coefficient may also prove a predominant factor under certain circumstances, such as in thin wood boards drying at low air velocity, its effect is usually not important in common kiln-drying conditions with high air velocity. As a result, most research has concentrated on determining the properties of the moisture diffusion coefficient. With the diffusion coefficient assumed constant, things become relatively simple due to the availability of the theoretical solution of the partial differential equation expressed by Fick's second law. However, past research results (Stamm 1964; Choong 1965; Moschler and Martin 1968; Ro-

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sen 1976) indicate that the moisture diffusion coefficient is not a constant, but rather a function of moisture content as well as diffusion direction. Therefore, only average values of diffusion coefficients can be derived from the unsteady-state drying curve.

In practice, three schemes (i.e., square-root, half-$\bar{E}$, and logarithmic methods) have been suggested for determining the average diffusion coefficient.

The square-root scheme, based on the equation derived by Boltzmann (Stamm 1964), is valid for short times:

$$D = \frac{\pi a^2(1 - \bar{E})^2}{4t} \quad (1)$$

In Eq. 1, $\bar{E}$, a, D, and t represent the fraction of evaporable moisture present in wood, half-thickness of a wood sample, diffusion coefficient, and drying time, respectively. The average diffusion coefficient derives from the slope of the curve when $(1 - \bar{E})$ is plotted versus $\sqrt{t}$ (Siau 1984).

The half-$\bar{E}$ scheme is based on Crank's (1975) suggestion that the average diffusion coefficient can be estimated by the value of D in Eq. 1 when $\bar{E} = 0.5$.

The logarithmic scheme, valid for long times (Crank 1975), is:

$$D = -\frac{4a^2}{\pi^2}\frac{d(\ln\bar{E})}{dt} \quad (2)$$

This equation can be derived from the theoretical solution of Fick's second law as shown in Eq. 3 under the equilibrium boundary condition (Skaar 1954), by truncating all terms except the first, taking the natural logarithm on both sides, and then differentiating the simplified equation. One can calculate the average diffusion coefficient from the slope of the curve when $\ln(\bar{E})$ is plotted versus t.

$$\bar{E} = (8/\pi^2)\sum_{n=1}^{\infty}\frac{1}{(2n-1)^2}\,e^{-\left(\frac{2n-1}{2a}\right)^2\pi^2 Dt} \quad (3)$$

Generally, these schemes have two major common characteristics. First, as approximate equations, only the first term in the infinite series was used in each equation. Although appropriate for a truly constant diffusion coefficient, few discussions in the literature (Crank 1975) justify the truncation procedure, or give the percent error due to such a procedure, when the diffusion coefficient is not a constant. Second, they are all subjective methods. For example, when using the square-root scheme, different people may obtain different slopes. This arises because the curve is usually not strictly straight, and therefore the portion taken as the straight line depends on personal preference. The decision-making may prove more difficult if relatively large experimental errors occur. In the half-$\bar{E}$ scheme, $\bar{E} = 0.5$ is obviously an arbitrary choice. Unless we know the exact form of a diffusion coefficient as a function of moisture content, there is no guarantee that $\bar{E} = 0.5$ is the best representative point for the calculation of average diffusion coefficient. Additionally, we generally expect the diffusion coefficients calculated from these three schemes to differ. In the square-root scheme, the diffusion coefficient is calculated from drying data when the moisture content is still high. In the logarithmic scheme, the diffusion coefficient is calculated when the moisture content is low.

In this paper, we suggest a new approach to calculating the average diffusion coefficient. Unlike other schemes, all data points are taken into account in the calculation, so that the calculated results represent average values of the diffusion coefficient. As an objective method, a given set of drying data will yield a unique answer. In addition, the error due to truncation in the other schemes will be greatly minimized. The average diffusion coefficient is an optimum one in the sense of the least-squares principle. Once the optimum average diffusion coefficient is found, the theoretical $\bar{E}$ value curve can accordingly be derived. Therefore, the effect of the deviation of the diffusion coefficient from a constant value can be examined by comparing the experimental data with the calculated curves. This scheme may be used conveniently in both theoretical analysis and routine calculation of an average diffusion coefficient.

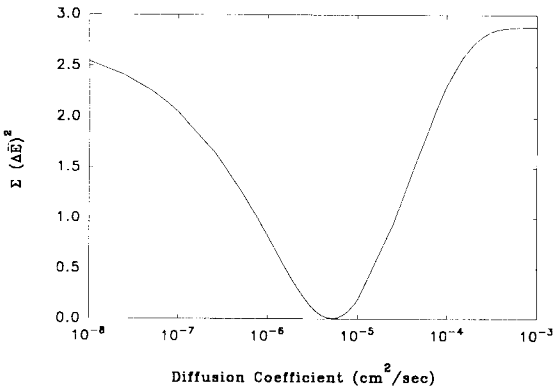

FIG. 1. Variation of sum of squares of $\bar{E}$ value difference as a function of diffusion coefficient.

OPTIMIZATION PROCEDURE

The basic equation used is Eq. (3), the theoretical Fourier series solution. If we select an arbitrary average diffusion coefficient, we can calculate a theoretical $\bar{E}$ for any time value. By studying the sum of squares of the differences of each experimental and theoretical $\bar{E}$ pair, we find that, as illustrated in Fig. 1, there exists a unique average diffusion coefficient at which the sum of squares of the $\bar{E}$ differences is minimized. We call this point the optimum average diffusion coefficient. To find this point, we can first set the expected lower and upper bound values of the diffusion coefficient. Then, we can locate the optimum average diffusion coefficient based on the golden section search principle (Fletcher 1980). This task would be tedious if attempted by hand; therefore, we developed a computer algorithm and wrote the FORTRAN program given in the appendix. In this program, all terms in the PARAMETER declaration can be adjusted according to each situation. The units of half-thickness are in centimeters. The ITEM value should be adjusted to the number of data points for each experiment. As reflected in the real variable declaration in the main program, the maximum number of data points is 30; however, this can be adjusted according to individual situations. The lower bound, upper bound, and optimum values of diffusion coefficients are output as the final results. The program can be executed in most 32-bit machines.

APPLICATION EXAMPLES

To illustrate the effect of the proposed scheme, we reanalyzed a part of Mamit's data (1983). The six hardwood species used in Mamit's experiment were dried from the fiber saturation point (FSP) to an equilibrium moisture content (EMC) of 12%. The environmental chamber, controlled at temperature 43 C and 45% relative humidity (RH), maintained an air speed of about 1.5 meters per second.

The graphs used to determine the average diffusion coefficients based on the square-root and the logarithmic schemes are given in Fig. 2. Obviously, one must decide which "straight" portion of a curve should be taken for the calculation of average diffusion coefficients. The calculated results given in Table 1 and Table 2 differ considerably, especially for the longitudinal direction.

The experimental values of $\bar{E}$ and the calculated curves based on the optimum average diffusion coefficients are shown in Fig. 3. In principle, we should not expect the curve to pass through all of the data points due to the fact that the curve is derived from the assumption that the diffusion coefficient is constant; however, the diffusion coefficient is generally a function of moisture content. The calculated curve passes through the optimum position where the sum of squares of $\bar{E}$ differences is minimized. The average diffusion coefficients based on the half-$\bar{E}$ scheme and the present optimum scheme are also given in Tables 1 and 2. When taking the calculated values of the present optimum scheme as a basis, we find the percent deviation of the half-$\bar{E}$ scheme from the one relatively small, with a maximum value of 12.8% in the longitudinal direction and 6.2% in the transverse direction. The percent deviations for the square-root scheme and the logarithmic scheme are relatively large, with maximum values of 170.6 and 45.3 for the square-root scheme and 62.5 and 27.5 for the logarithmic scheme in the longitudinal direction and the transverse direction, respectively. These comparisons support Crank's suggestion that calculated diffusion coefficients based

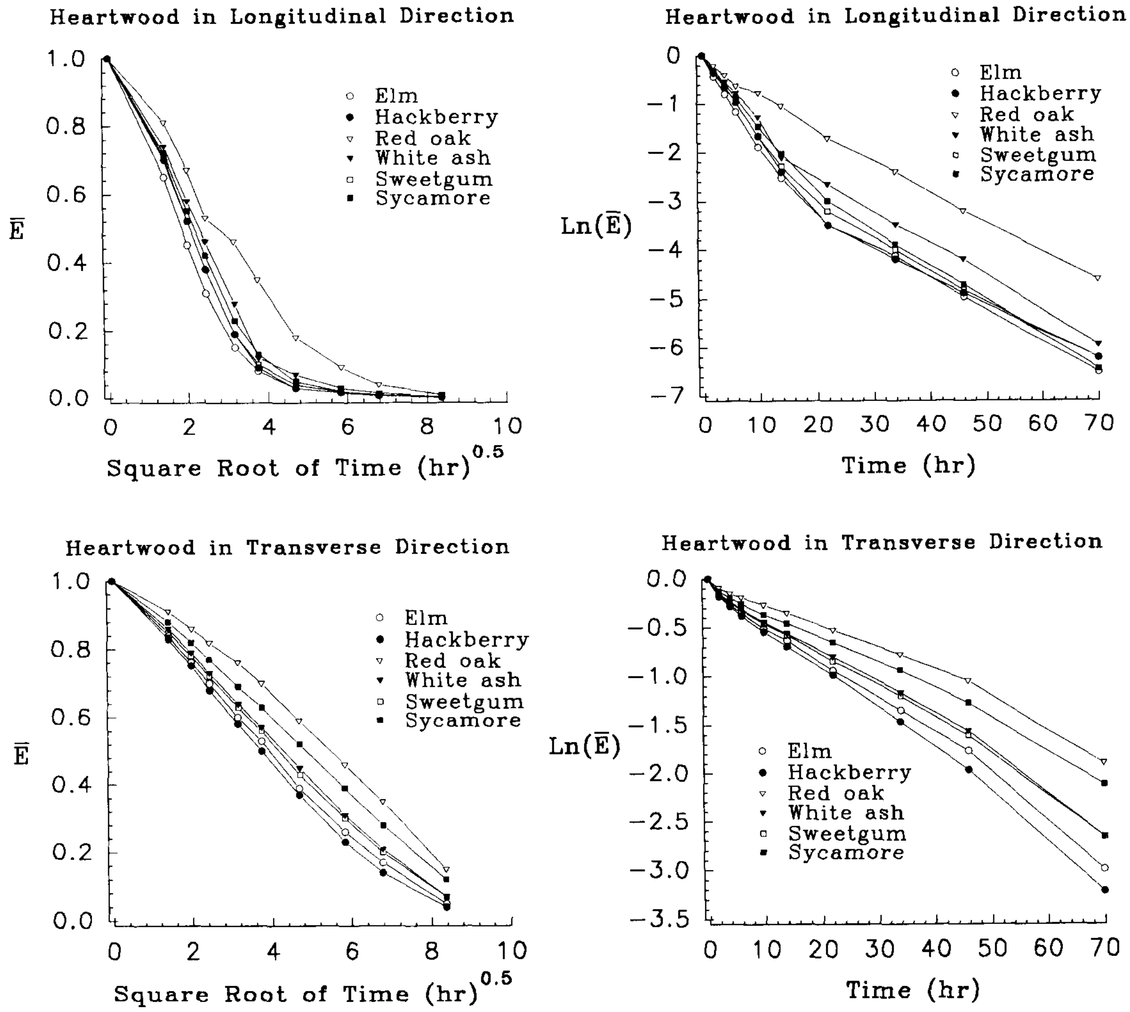

FIG. 2. Relationship between Ē and the square root of time, and between natural logarithmic Ē and time.

TABLE 1. *Comparison of heartwood diffusion coefficients calculated by four methods.*

Direction:	Longitudinal				Transverse			
Method:	SQRT*	LOG	HALF-Ē	OPTIMUM	SQRT*	LOG	HALF-Ē	OPTIMUM
	$\times 10^{-6}$ cm^2/sec							
Elm	40.91	11.01	25.13	27.89	5.98	6.38	5.60	5.92
Hackberry	33.47	10.49	20.53	23.37	7.35	7.17	6.28	6.50
Red oak	14.08	11.38	11.40	11.13	3.85	3.90	2.90	3.06
White ash	45.55	11.65	16.49	18.61	5.12	5.62	4.71	5.01
Sweetgum	32.84	12.18	20.53	23.02	5.58	5.77	4.97	5.23
Sycamore	31.54	12.97	18.45	20.57	4.55	4.53	3.69	3.92

* Results from Mamit's thesis (1983).

TABLE 2. *Comparison of sapwood diffusion coefficients calculated by four methods.*

Direction:	Longitudinal				Transverse			
Method:	SQRT*	LOG	HALF-$\bar{E}$	OPTIMUM	SQRT*	LOG	HALF-$\bar{E}$	OPTIMUM
	$\times 10^{-6}$ cm^2/sec							
Elm	30.70	11.01	17.87	19.48	5.53	6.01	4.97	5.31
Hackberry	35.00	9.11	21.28	24.29	5.92	5.50	4.81	5.09
Red oak	21.68	12.18	15.08	13.86	5.13	4.14	3.31	3.53
White ash	39.15	11.38	13.12	14.47	5.54	5.30	4.50	4.69
Sweetgum	47.01	10.49	16.82	19.29	5.45	5.60	4.81	5.06
Sycamore	26.09	13.19	13.65	15.25	5.09	4.78	4.50	4.34

* Results from Mamit's thesis (1983).

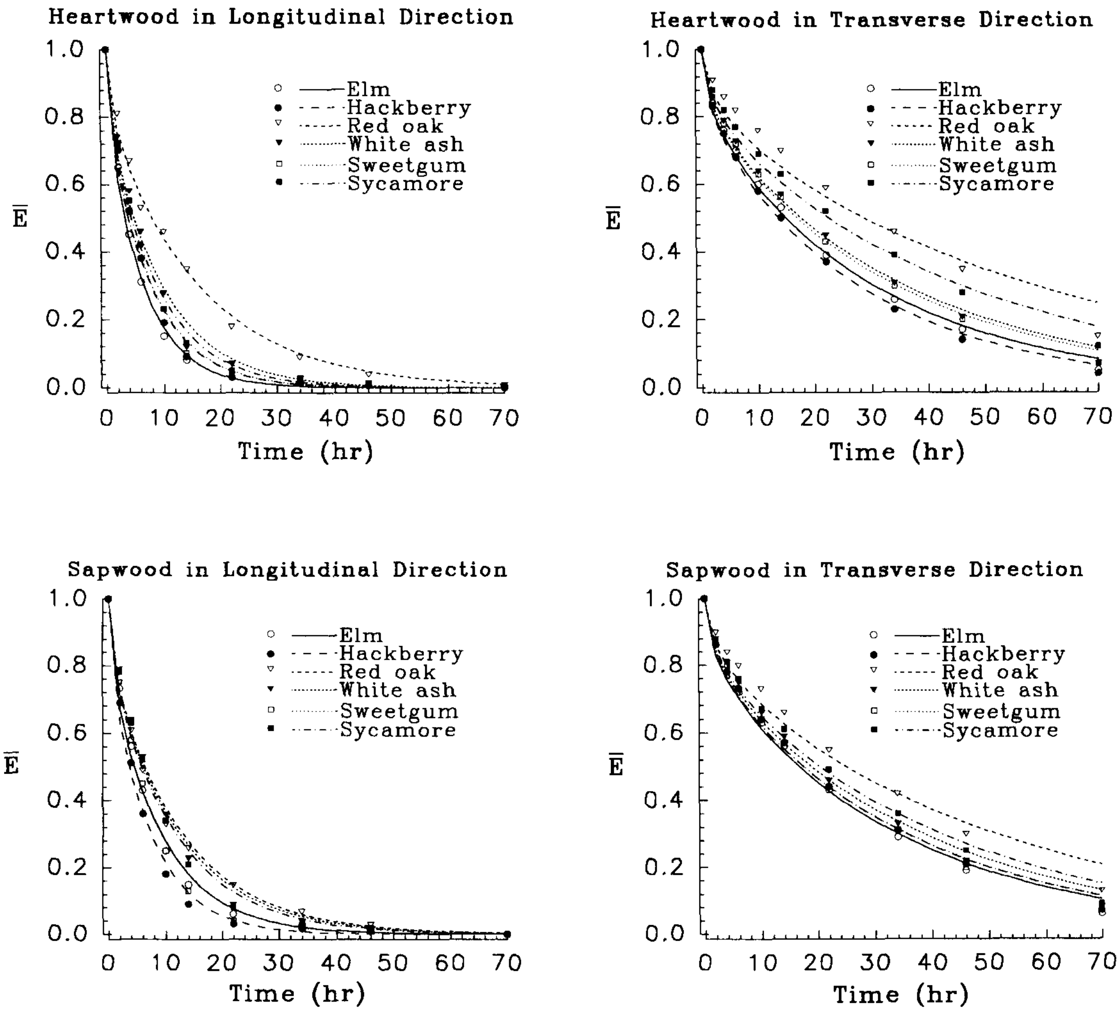

FIG. 3. Comparison of predicted and measured $\bar{E}$ values as a function of drying time (lines correspond to the theoretical $\bar{E}$ values).

on the half-$\bar{E}$ scheme give some average values, though not optimum ones.

When examining the relationship of the experimental data to the calculated curves in the longitudinal direction in Fig. 3, we find an interesting phenomenon. For most heartwood and some sapwood samples, in the longitudinal direction but not in transverse direction, the theoretical curves fitted the data points quite satisfactorily. This implies that the diffusion coefficients in the longitudinal direction may virtually be a constant, whereas those in the transverse direction usually are not.

DISCUSSION AND CONCLUSIONS

Based on the golden section search principle, an optimization procedure was developed to find the optimum average diffusion coefficients using the Fourier series solution as a basic equation. This scheme can fully utilize the data and give the optimum values of average diffusion coefficients objectively, with very small truncation errors, and may be used as an objective basis for comparisons of experimental results obtained by different researchers. It may be used not only as a research tool to reveal the basic mechanism of moisture transport in woods in a theoretical study, but in routine calculations as well.

One must be cautious when applying this scheme. The assumption that the value of $\bar{E}$ at the surface immediately drops to zero when drying begins should hold. If not, an error due to the neglect of surface resistance will result. In the example of Mamit's data, the air velocity is less than the critical value, as suggested by Rosen (1978); therefore, we expect that some errors due to surface resistance may already be confounded in the calculation. Several approaches have been suggested to estimate the magnitude of surface resistance (Choong and Skaar 1969, 1972; Liu 1989), and a more complex computer algorithm should be developed to calculate the moisture diffusion coefficients and surface emission coefficients objectively. The present optimum scheme has shown a more systematic and objective way to conduct data analysis in wood drying than previously available.

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APPENDIX

FORTRAN PROGRAM FOR LOCATING OPTIMUM AVERAGE DIFFUSION COEFFICIENT

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*  THIS PROGRAM CAN BE USED TO FIND THE OPTIMUM UNIDIRECTIONAL DIF-
*    FUSION COEFFICIENT OF A RECTANGULAR SAMPLE UNDER THE ASSUMP-
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*    TION THAT SURFACE RESISTANCE IS NEGLIGIBLE. GOLDEN SECTION SEARCH
*    PRINCIPLE WAS APPLIED TO FIND THE OPTIMUM DIFFUSION COEFFICIENT
*    BASED ON THE LEAST SQUARES CRITERION.
*
*  VARIABLE LIST
*  HLFT --- HALF THICKNESS OF A SAMPLE IN CENTIMETER
*  DL --- LOWER BOUND OF CHOSEN DIFFUSION COEFFICIENT
*  DU --- UPPER BOUND OF CHOSEN DIFFUSION COEFFICIENT
*  ITEM --- NUMBER OF DATA POINTS, WHICH CAN BE ADJUSTED
*  TSN --- TIME ARRAY SUBSCRIPT
*  DSN --- DIFFUSION COEFFICIENT ARRAY SUBSCRIPT
*  TIME --- DRYING TIME ARRAY
*  REALE --- E CALCULATED FROM MEASURED DATA
*  CALCE --- E CALCULATED FROM TRIAL DIFFUSION COEFFICIENTS
*  SS --- SUM OF SQUARES OF THE DIFFERENCE BETWEEN REALE AND CALCE
*  DIFF --- DIFFUSION COEFFICIENT ARRAY
*  OPTDF --- OPTIMUM DIFFUSION COEFFICIENT
*
*  ..... DECLARATIONS .....
      PARAMETER (HFLT=1.27,DL=1.E-8,DU=1.E-4,ITEM=10)
      INTEGER TSN, DSN
      REAL TIME(30),REALE(30),CALCE(4,30),SS(4),DIFF(4),OPTDF
*
*  ..... READ MEASURED DATA IN .....
      READ *,(TIME(I),REALE(I),I=1,ITEM)
*
*  ..... CALCULATE DIFFUSION COEFFICIENTS .....
      DIFF(1)=DL
      DIFF(2)=DU
      DIFF(3)=DIFF(1)+(DIFF(2)-DIFF(1))*.381966
      DIFF(4)=DIFF(1)+(DIFF(2)-DIFF(1))*.618034
*
*  ..... CALCULATE SUM OF SQUARES .....
      DO DSN=1,4
        DO TSN=1,ITEM
          CALCE(DSN,TSN)=SUMMTN(HFLT,TIME,DIFF,TSN,DSN)
        ENDDO
        CALL SUMSQ(SS,REALE,CALCE,DSN,ITEM)
      ENDDO
*
*  ..... CALCULATE OPTIMUM DIFFUSION COEFFICIENT .....
      DO WHILE ((DIFF(2)-DIFF(1)).GT.1.E-10)
        IF (SS(3).GT.SS(4)) THEN
          DIFF(1)=DIFF(3)
          DIFF(3)=DIFF(4)
          DIFF(4)=DIFF(1)+(DIFF(2)-DIFF(1))*.618034
          SS(1)=SS(3)
          SS(3)=SS(4)
```

```
          DSN=4
          DO TSN=1,ITEM
            CALCE(DSN,TSN)=SUMMTN(HLFT,TIME,DIFF,TSN,DSN)
          ENDDO
          CALL SUMSQ(SS,REALE,CALCE,DSN,ITEM)
        ELSE
          DIFF(2)=DIFF(4)
          DIFF(4)=DIFF(3)
          DIFF(3)=DIFF(1)+(DIFF(2)-DIFF(1))*.381966
          SS(2)=SS(4)
          SS(4)=SS(3)
          DSN=3
          DO TSN=1,ITEM
            CALCE(DSN,TSN)=SUMMTN(HLFT,TIME,DIFF,TSN,DSN)
          ENDDO
          CALL SUMSQ(SS,REALE,CALCE,DSN,ITEM)
        ENDIF
      ENDDO
*     OPTDF=(DIFF(1)+DIFF(2))/2.
*
* ..... PRINT OUT RESULTS .....
      PRINT *, 'LOWER BOUND OF DIFFUSION COEFFICIENT:',DIFF(1)
      PRINT *, 'UPPER BOUND OF DIFFUSION COEFFICIENT:',DIFF(2)
      PRINT *, 'OPTIMUM AVERAGE DIFFUSION COEFFICIENT:'OPTDF
      STOP
      END
*
* ---------------------------------------------------
      FUNCTION SUMMTN(HLFT,TIME,DIFF,TSN,DSN)
*
* AVERAGE E IS CALCULATED BASED ON THEORETICAL FOURIER SERIES SO-
*   LUTION OF DIFFUSION EQUATION.
*
* ..... DECLARATIONS .....
      INTEGER TSN,DSN
      REAL TIME(*),DIFF(*)
      REAL CTERM,EXPTM,TERM
*
* ..... INITIALIZATION .....
      SUMMTN=0.
      TERM=1.
      I=0
*
* ..... CALCULATE AVERAGE E .....
      DO WHILE ((I.LT.100).AND.(TERM.GE.1.E-30))
        I=I+1
        CTERM=8./ACOS(-1)**2/(2.*I-1.)**2
        EXPTM=(2.*I-1.)**2/4.*ACOS(-1)**2/HLFT**2
```

```
     +          *3600.*TIME(TSN)*DIFF(DSN)
          IF (EXPTM.GT.100.) EXPTM=100.
          EXPTM=EXP(-EXPTM)
          TERM=CTERM *EXPTM
          SUMMTN=SUMMTN+TERM
        ENDDO
        RETURN
        END
*
* ------------------------------------------------
        SUBROUTINE SUMSQ(SS,REALE,CALCE,DSN,ITEM)
*
* SUM OF SQUARES IS CALCULATED FOR A DIFFUSION COEFFICIENT
*
* ..... DECLARATIONS .....
        INTEGER DSN,ITEM
        REAL REALE(*),CALCE(4,*),SS(*)
        REAL ISS
*
* ..... CALCULATE SUM OF SQUARES .....
        LSS=0.
        DO I=1,ITEM
          LSS=LSS+(REALE(I)-CALCE(DSN,I))**2
        ENDDO
        SS(DSN)=LSS
        RETURN
        END
```