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A COMMENT FROM THE EDITOR ON THE FOLLOWING PAPER BY PROFESSOR HART:

I have procrastinated for sometime on commenting about my thoughts on how we (as a Society) can more effectively use the *Professional Affairs* section of *Wood and Fiber*. Time for action!

The following article by Dr. Hart is an example of one such use (my opinion). Dr. Hart would like this information put to use by some of your researchers out there, and the article provides plenty of details but not much theory. As with all articles in *Wood and Fiber*, this paper has been peer reviewed and page charges will be charged to the author.

The only presentations in Professional Affairs that are "charged" to the Society are the pages devoted to the business of the Society (Referral Service, annual meeting business, book reviews, and related items).

Volume 11, No. 4, contained two excellent examples of what I believe to be needed items for the Society membership and indeed are "at home" in *Professional Affairs*. These were the articles by Helmuth Resch and by H. M. Barnes.

We need to put this section of *Wood and Fiber* to greater use! How many other journals, of professional societies, do you know of where the opportunity to publish on research, philosophy, teaching, extension, etc., exists? I welcome your thoughts on this subject of expanding usage of the *Professional Affairs* section of our journal.

Sincerely,

E. Allen McGinnes, Jr.
Editor, *Wood and Fiber*

SIMSOR: A COMPUTER SIMULATION OF WATER SORPTION IN WOOD[1]

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ABSTRACT

SIMSOR, a computerized simulation of sorption, represents an effort to structure the known essential physical phenomena that control the drying behavior of wood in such a way as to permit the duplication, with acceptable accuracy and cost, of experimental data obtained from actual drying studies. Programming knowledge is not required for its use. It can accurately simulate a typical red oak kiln schedule in less than one minute of computer time. It will handle adsorption or desorption, from freezing temperatures to boiling temperatures, and at humidities from virtually 100% to nearly 0%. Wood of any thickness and density, permeable or impermeable, can be simulated over any desired range of wood moisture content. However, its use to duplicate experimental data requires that the diffusion coefficient be adequately defined over the entire applicable range of moisture contents. At present, this will generally require a trial-and-error approach, especially in the free water range. Free water is treated the same as bound water, but the temperature dependence may be canceled, if desired.

Although the simulation has already been proven under a variety of trials, it still needs to be tested under the widest possible range of applications. Wherever duplication of experimental data proves the validity of the simulation, it can then be used to provide a much more comprehensive analysis of wood-drying procedures and variables, and in far less time at far less cost, than is possible by actual physical trials.

Keywords: Computer simulation, drying simulation, kiln drying simulation, moisture movement, sorption.

INTRODUCTION

When wood is drying, water vapor is transferred from the wood surface to the air stream, moisture moves from within the wood to the surface, and heat is transferred from the air stream to the wood. SIMSOR is a computer simulation of sorption that continuously balances all of these interdependent phenomena. It does so for adsorption or desorption, at air temperatures ranging from the freezing point of water to its boiling point, at air relative humidities from virtually 100% to nearly 0%, for wood moisture contents ranging from total saturation to nearly 0%, and it does so for any desired wood thickness and specific gravity. Only minimal mathematical effort is necessary for its use. A knowledge of computer programming, while always helpful, is not required. In fact, to encourage the widest possible use of the program, every effort has been made to provide for data input that permits a maximum versatility in the application of the program without the necessity for internal alterations that require programming knowledge.

The potential benefits to be gained from the use of SIMSOR are substantial. The user will be able to estimate the effect upon drying time of a variety of interrelated factors such as air velocity, dry and wet bulb temperatures, kiln schedule alterations and interruptions, lumber thickness, and both the average level and the shape of the initial moisture profile. The simulation will greatly aid in the search for the combinations of controllable variables that result in the least cost and the least consumption of energy. The fact that SIMSOR provides a precise moisture profile from the wood surface to the center should make it feasible to assess the stress levels and the associated degrade risks that will result from proposed drying schedules. And in view of the short computer time required by the program, SIMSOR may even find a place in the day-to-day control of industrial dry kilns. But the greatest value of SIMSOR may come from the improved depth and breadth of understanding that it should provide for the drying specialist both in research and in production.

BASIC DESIGN

SIMSOR simulates the behavior of a single wood specimen (a slab), that is, a single moisture profile from the surface to the center of the wood, when the wood is exposed to one or more specified sets of environmental conditions, such as a dry kiln schedule. Subsequent publications will cover expansion of the simulation to encompass as many locations (profiles) as desired across an entire stack of lumber, as well as the use of continuously changing schedules and also the use of weather data input for air drying simulation. Since all of these applications require internal programming alterations, it is necessary to employ separate programs for them. SIMSOR is the basic program from which all of these applications can be readily developed.

SIMSOR is a finite difference solution of the wood moisture profile across the board thickness during sorption, but coupled to the heat and vapor transfer between the wood surface and the air. The rate of vapor transfer at the surface is directly proportional to the difference in vapor pressure between the air and the wood surface. The rate of heat transfer between the air and the wood surface is directly proportional to the temperature difference between them. The temperature of the wood is assumed to be uniform from the surface to the center. The surface to center moisture profile across the wood is divided into a specified number (N) of equal-sized cells (*cells* has no connection whatsoever with *wood cells* in the anatomical sense). The rate of moisture diffusion between adjacent cells is directly proportional to their moisture content difference and to the diffusion coefficient (Siau 1971), adjusted to the saturated vapor pressure of water at the temperature of the wood (Stamm 1964). The dependence upon the saturated vapor pressure to reflect the effect of changing wood temperatures is built into the program but may be canceled above a freely specified moisture level (TDL) if desired. The diffusion coefficient across the moisture profile may be varied (by the user of the program) with the moisture content of each cell as desired.

Other investigators, such as Moschler and Martin (1968), Peck and Kauh (1968), Kawai et al. (1978), Bramhall (1979), and Ashworth (1978), have applied simulations to the drying of wood. All of these dealt with softwoods (except Peck and Kauh dealt with balsa) and all, including SIMSOR, differ from one another in some fundamental respects although all share many similarities.

TABLE 1. *A duplication of the input data print-out for the computer simulation plotted in Fig 1. Each row beneath the variable names represents a data input card.*

Column → 11	21	31	41	51	61	71
ID	DESCR(I)					
1	DUPLICATION OF FPL KILN DRYING SCHEDULE - MANUAL FIG. 101					DAY
SG	A	N	TW	TWDLT	TDL	
.58	1.3	30	110.	5.	500.	
DST	TSD	BWDM	CBWDM	RBWDM		
.53D-01	104.	1.8	22.	44.		
FWL	FWDBL	FWDM	CFWDM	RFWDM		
500.	1.8	0.5	55.	10.		
RHSH	EMCSH	RHSL	EMCSL	TSEMC	B	
.80	15.8	.40	7.4	80.	14.43	
IWRT	WRT	FINIS	JJ		NCLM(I)	
1	1.	0.0	80000		1 2 4 7101418222630	
TDBS(I)	TWBS(I)	NSD(I)	TEST(I)	QRATES(I)	TSQS(I)	
110.	106.	-1	51.0	.7854D-02	106.	
110.	105.	-1	41.3			
110.	102.	-1	34.5			
110.	96.	-1	31.0			
120.	90.	-1	26.0			
130.	80.	-1	19.3			
140.	90.	-1	11.5			
180.	130.	-1	7.0			
180.	145.	-1	6.0			
180.	172.	2	1.0			
(blank card)						
C(J)	C(J)	C(J)	C(J)	C(J)	C(J)	C(J)
81.						
(blank card)						
blank card or ID card for the next data set						

APPLICATION EXAMPLE

Figure 1 illustrates the application of SIMSOR to the data for a red oak kiln run as depicted in Figure 101 of the FPL's Dry Kiln Operator's Manual, using schedule T4, D2 (Rasmussen 1961). It shows the fit of the simulation curve to the actual data points at the end of each kiln step. All differences between them were less than 1% MC. Less than one minute of computer time (CPU = 0:38.8 on an Amdahl Model V7, executed in 50 kilobytes of core memory, using IBM Fortran IV) was required for the completion of this entire simulation.

Table 1 shows the input data variables for Fig. 1 as punched by the user. Above each is the name of the variable as provided by the computer print-out. The definitions of these variables are given in the following list.
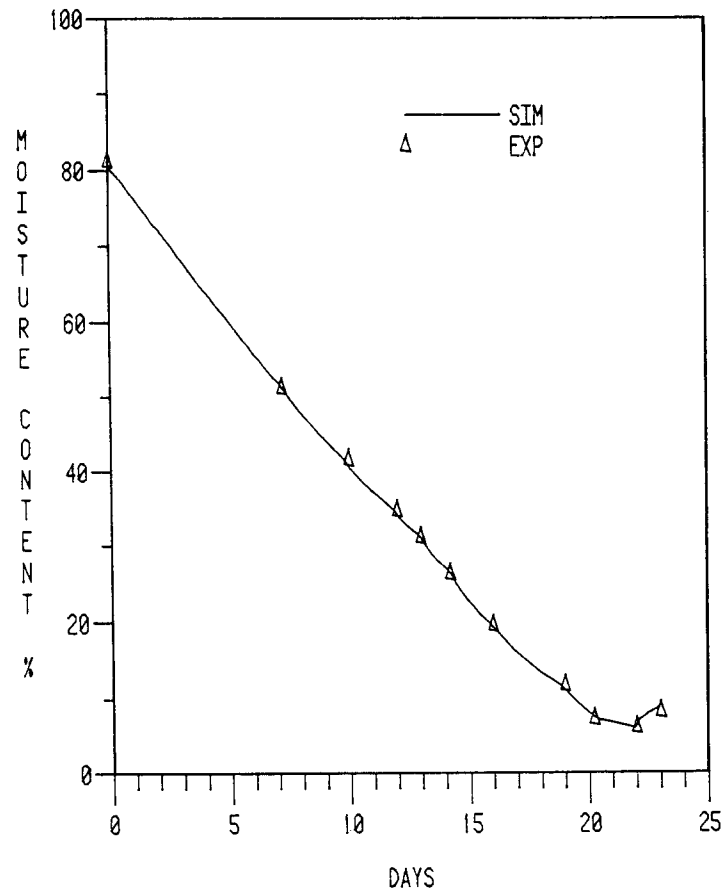
FIG. 1. A moisture content versus time plot showing the fit of the simulated curve to the red oak experimental data points at the end of each kiln step (experimental data taken from Fig. 101 of the FPL Kiln Drying Manual (Rasmussen 1961)).

Input Variables

Card 1

ID	Identification number
DESCR(I)	Description

Card 2

SG	Specific gravity (dimensionless) (o.d. wt./green volume recommended)
A	Specimen half-thickness (cm) (same volume basis as SG)
N	Number of cells in the moisture profile (105 maximum)
TW	Temperature of the wood (°F), initial value
TWDLT	Maximum permissible wood temperature change per loop (°F)
TDL	Temperature-dependent-limit (% MC)

Card 3

D$T	Diffusion coefficient (cm²/time)
T$D	Temperature at which D$T is defined (°F)
BWDM	Bound water diffusion multiplier (dimensionless)
CBWDM	Center bound water diffusion multiplier (% MC)
RBWDM	Range bound water diffusion multiplier (% MC)

Card 4

FWL	Free water limit (% MC)
FWDBL	Free water diffusion base line (dimensionless)
FWDM	Free water diffusion multiplier (dimensionless)
CFWDM	Center free water diffusion multiplier (% MC)
RFWDM	Range free water diffusion multiplier (% MC)

Card 5

RVP$H	Relative vapor pressure high value (dimensionless)
EMC$H	Equilibrium moisture content high value (%)
RVP$L	Relative vapor pressure low value (dimensionless)
EMC$L	Equilibrium moisture content low value (%)
T$EMC	Temperature at which the two RVP-EMC points are defined (°F)
B	Barometric pressure (psi)

Card 6

IWRT	Code defining the dimensions of WRT (1 = % MC, 2 = time)
WRT	Write interval for print-out (% MC or TIME UNIT)
FINIS	Difference between average profile MC and EMC which terminates the run (% MC)
JJ	Maximum number of main or outer loops (iterations) for terminating the run
NCLM(I)	The ten cells of the profile which are to be printed out

Card 7A . . .

TDBS(I)	Temperature dry bulb step (°F) for the ambient air
TWBS(I)	Temperature wet bulb step (°F) for the ambient air
NSD(I)	Code defining the dimensions and functions of TEST(I)
	−1: TEST(I) is a % MC limit and a lower test (desorption)
	0: TEST(I) is a TIME INTERVAL and no sorption occurs
	1: TEST(I) is a % MC limit and an upper test (adsorption)
	2: TEST(I) is a TIME INTERVAL (adsorption or desorption)
TEST(I)	Test level which initiates transfer to the next step (% MC or TIME)
QRATES(I)	Surface transfer coefficient (g cm⁻² time⁻¹ °F⁻¹) (A given value will be duplicated in subsequent steps if undefined there.)
T$QS(I)	Temperature at which QRATES(I) is defined (°F) (also duplicates)

Card 8A . . .

C(J)   Initial moisture contents of the profile cells from the surface,
                     C(1), to the center, C(N). One to N values may be specified
                     since a zero or blank value will result in the preceding value
                     being duplicated to define the remainder of the N values.
                     (C(J) = % MC = 100% × water weight/oven-dry wood weight.)

Beneath each row of variable names in Table 1 is a row of input data repre-
senting a punched card (all are numerical data except the description, DESCR).
For simplicity, ten spaces or columns (one blank and nine used spaces) were
allocated for each of the variables on each card with the first ten spaces of each
card left unused, except for the ID number on the first card. The only other
exceptions to the spacing are with DESCR, which occupies the last 69 spaces of
its card, and with NCLM, where two spaces per cell are used to define the ten
cells to be printed. Decimal numbers may be located anywhere in their allotted
nine spaces, but the exponents, if present (D$T and QRATES), must be right
justified, as must the nondecimal (integer) variables (ID, N, IWRT, JJ, NCLM,
NSD).

Card 1. The ID must be integer numbers only. It cannot be blank or zero since
this signifies that no data set follows. The description, DESCR, should include
the unit of TIME to be employed in the data. Any desired unit may be used (days,
hours, minutes, etc.) but must be consistently used for all time-defined input data
(i.e. D$T, WRT if IWRT = 2, TEST if NSD = 0 or 2, and QRATES). The output
data will be in this time unit.

Card 2. Both SG and A remain constant (no attempt has been made to account
for shrinkage) so green dimension (and oven-dry weight) values would be pref-
erable, at least in the USA. While space for N = 105 is provided, N = 30 is
recommended for the number of profile cells for excellent accuracy at reasonable
cost. However, for preliminary trials, N = 10 gave values almost within 1% MC
of the N = 30 values and required only about half the CPU time (0:17.5 vs.
0:38.8). The initial value of TW, the wood temperature, is important in its effect
on the initial sorption rate. If it is below the dew point of the ambient air, con-
densation on the wood will be simulated as the wood heats up regardless of how
wet or dry the wood is. TWDLT limits the magnitude of change in TW that is
permitted in a single loop or iteration. A value of 5 F is recommended. Some
restriction on the wood temperature change per loop is necessary to prevent
inaccurately large changes after sudden changes in ambient air temperature (e.g.
putting a very cold charge of lumber into a hot kiln). TDL, the last value on the
second card, is the moisture content above which the rate of diffusion is not
dependent upon the saturated vapor pressure at the wood temperature. This
permits the free water to be treated differently from the bound water, if desired.
However, in the examples herein, TDL was set to a high value to insure that all
water was treated the same.

Card 3. This card and card 4 are for data which the user must supply to permit
defining of the diffusion coefficient at any temperature and any moisture content
encountered during the simulation. The user of SIMSOR must specify the base
diffusion coefficient, D$T, and the temperature, T$D, at which it is defined. The
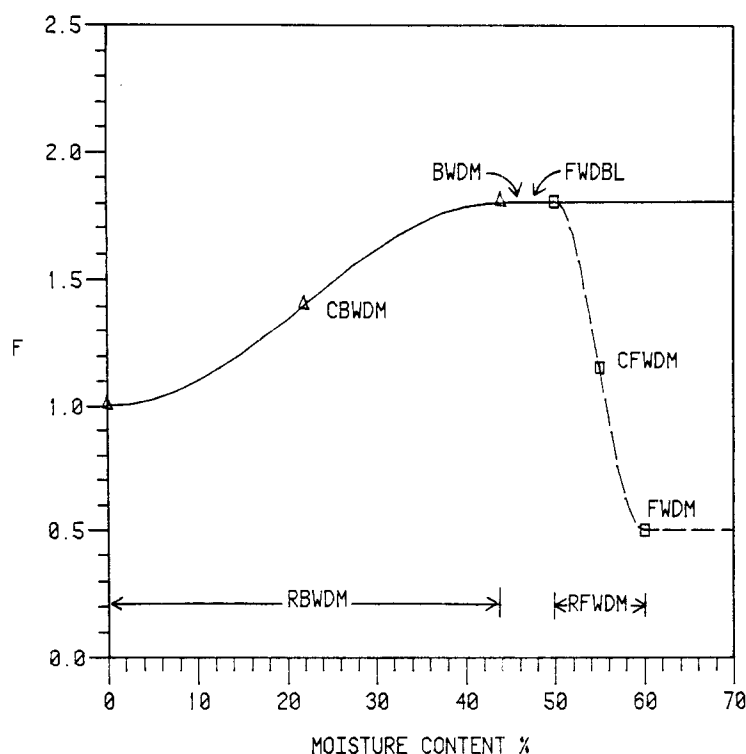
FIG. 2. The multiplier, F, used for changing the diffusion coefficient with moisture content to obtain the simulated curve in Fig 1. The dashed curve was not used.

computer will automatically adjust this coefficient to any other temperature encountered (in proportion to the saturated vapor pressure of water). However, the diffusion coefficient also changes with moisture content. Since no universally applicable function for the moisture effect is known, the program user must either use the supplied procedure or define his own function. This equation must define a value, F(I), for each and every cell moisture content, C(I), so that in the computer, the base diffusion coefficient, D$T, can be multiplied by F(I) to correct it to the desired value for each cell moisture content encountered. Initial estimates of D$T and of its change with moisture content may be arbitrarily selected on a trial and error basis or may be obtained from evaluation of experimental data or from the literature. Stamm (1964) has calculated theoretical values that can be tested for use in the bound water range. His model also shows the effect of specific gravity. His diffusion coefficients are very nearly inversely proportional to specific gravity raised to the 2.25 power so this provides a useful estimate of the specific gravity effect. SIMSOR does not change the diffusion coefficient with changes in specific gravity so this must be done by the user.

A purely arbitrary but flexible procedure for defining an equation to calculate F has been included in the program. It is simply a technique to provide the user with substantial flexibility in making his choice of values, but he can do so without internal program alterations. (Those who do not mind altering the program can insert any other functions they wish.) Figure 2 illustrates the curve that gave the

computer curve fit to the data shown in Fig. 1. It is an S-shaped transition (a sine curve) from one constant level of F, unity, at low moisture content to a second constant level, BWDM, at a higher moisture content. The curve is centered at moisture content CBWDM and reaches CBWDM ± RBWDM/2 as the upper and lower moisture content limits of the S-curve. Below the lower limit the multiplier is unity and above the upper limit it is BWDM. These data for F(I) are printed out by the computer for ease of plotting, if desired. For the data in Table 1, the F multiplier for D$T increases from unity at 0% MC to 1.4 at 22% MC (1.4 = (1 + 1.8)/2) and to 1.8 at 44% MC. It remains at 1.8 above 44%. In general, it may prove desirable to keep the range, RBWDM, equal to twice the center value, CBWDM, when possible since this results in one less variable to manipulate in trying to fit specified experimental data. However, any desired values can be used, and BWDM can be less than unity, thus decreasing D$T with increasing moisture if desired. Although unlikely for bound water, a reduction of D$T for the free water of impermeable woods may prove desirable.

Card 4. To permit such flexibility, a second S-shaped curve is defined on this card. It is similar to the previous curve in that FWDM is the level of F(I) at the higher moisture content end, with the curve centered at CFWDM and reaching CFWDM ± RFWDM/2. But FWL defines the moisture content above which this curve will be utilized (i.e. the switchover point from the bound water curve to the free water curve) and, while unity is the base line for the bound water curve, FWDBL defines any desired value as the base line for the free water curve. Thus if the entire S-curve is above FWL (it need not be), then F(I) varies from FWDBL at the lower moisture content end to FWDM at the higher moisture content level. Suppose, for example, that in Fig. 2 it is desired to reduce F(I) from its 1.8 value to a value of 0.5 as the moisture content, C(I), increases from 50% to 60%. Then FWL = 44.0 (any value from 44 to 50 would suffice), FWDBL = 1.8, FWDM = 0.5, CFWDM = (50 + 60)/2 = 55, RFWDM = 60 − 50 = 10. This curve, which is shown in Fig. 2, was actually ignored by SIMSOR since FWL = 500.0 was used rather than 44.0, so the transfer point is beyond the initial moisture content of the wood. The use of these sine curves is more cumbersome to describe than to actually apply. They do offer a systematic way to achieve flexibility in defining the change in diffusion coefficient with changing moisture content, and any values whatsoever may be employed to obtain the desired values of F.

Card 5. This card defines the two parameter RVP-EMC isotherm employed in the program (Hart 1977). The two pairs of values, plus T$EMC, are sufficient to define the isotherm for all temperatures between (but not including) 0 F and 250 F (the program will run only within these temperature limits). Values may be obtained from a standard reference (e.g., Forest Products Laboratory 1974; Smith 1963) or, for experimental data in which the EMC was determined, the experimental data can be used. This permits the simulation to approach the actual observed specimen EMC rather than a standard published value. If only one experimental value is available, then a good procedure is to calculate a second value that has the same ratio to the standard value as does the observed value. The barometric pressure completes the psychrometric data since it is a part of the psychrometric equation. There is no need for it to reflect daily fluctuations. Most published tables simply use the standard sea level value (14.69 psi), but it

should be corrected for altitude. The value in Table 1 is for the standard value corrected to an altitude of 500 feet (Weast 1973).

Card 6. The values on this card serve to control the print-out of the computed data and may control the length of the run. WRT tells the computer how often to print out its progress and IWRT tells it whether to do so on an elapsed moisture content or an elapsed time basis. If WRT = 0.0, every main loop will be printed since the elapsed moisture content or time will exceed zero. FINIS tells it how close the average MC can get to the EMC (equilibrium moisture content) before the run will be terminated. Just as in actual drying, it becomes quite expensive to run too close to EMC since sorption becomes so slow. In the Table 1 example, however, the cut-off was in the control of the step schedule so 0.0 was permissible for FINIS. JJ, the maximum permissible number of repetitions of the main or outer loop (J loop), may also be used to terminate the run and is especially useful for preliminary trials. In Table 1, the very large value insured that it would not be used for terminating the run. NCLM is used to select ten cells across the profile for print-out. The first and last cells will probably always be desired but intervening selections depend upon the individual need. For example, if surface stresses are of interest, then the moisture contents of the cells close to the surface may be of primary interest. Remember to change NCLM if N is changed.

Card 7A . . . Up to 99 step cards (more if the program is altered) can be used to define any sequence of environmental conditions to which the wood is to be exposed. The listing of the ambient dry bulb temperature (TDBS), the wet bulb temperature (TWBS), and the moisture content (TEST) at which the ambient conditions will be changed to the next step differs slightly from a conventional kiln schedule listing. TEST is the moisture content at which control is transferred *out* of the step rather than *into* the step as with conventional listings. The last step card must be blank or zero in the TDBS space to indicate the end of the step cards. QRATES and T$QS need be indicated only on the first card since they will be automatically adopted for subsequent steps unless a new value is indicated.

For a given air velocity, the surface transfer coefficient, QRATES, is simply the maximum possible sustained drying rate, the wet bulb rate, divided by the wet bulb depression. Thus QRATES is a property of the air stream rather than of the wood itself. Fast drying species such as yellow poplar and southern pine sapwood often dry at a constant rate early in the drying run (see Fig. 2 of Hart and Darwin 1971). During this period they are drying like a wet bulb and at the wet bulb temperature (thus TW = TWB). The observed drying rate (g cm^{-2} time^{-1}) divided by the known wet bulb depression then gives QRATES (g cm^{-2} time^{-1} °F^{-1}) at T$QS (°F), which is equal to the wet bulb temperature. This surface transfer coefficient is slightly temperature-dependent, hence, the necessity for T$QS. When dealing with slow drying species which may never exhibit a constant rate period, it is well to include fast drying specimens for the sole purpose of obtaining data for the determination of QRATES. (These specimens may require prior soaking in water to insure adequate wetness.) If necessary, QRATES may also be obtained from published data. After conversion to the dimensions employed herein (g cm^{-2} days^{-1} °F^{-1}), the results of Stevens et al. (1956) result in the equation

$$QRATES = 0.0218 + 0.000092V \qquad \text{at } 122.4 \text{ F} \qquad (1)$$

while those of McNamara (1969) gave

$$QRATES = 0.0119 + 0.000138V \qquad \text{at } 94.8 \text{ F} \qquad (2)$$

where V = air velocity in feet/minute. But since, for use of these equations, the air speed must be measured and the effectiveness may be strongly controlled by the degree of laminar versus turbulent air flow, drying rate data taken from rapidly drying permeable wood exposed to the actual drying conditions are probably the safest source. Figure 3 shows the drying curves of ½-inch-thick yellow poplar and white oak (from Hart and Darwin 1971) dried under identical conditions, with the QRATES (0.0466 g cm^{-2} days^{-1} °F^{-1}) (at 94.8 F) obtained from the constant rate portion of the poplar data. The simulation was fitted to these diverse specimens with less than 1% moisture content difference between simulated and experimental data points. Below 30% MC, the differences were less than 0.5% MC.

For the sake of illustration, it was assumed that the oak in Fig. 1 dried like a wet bulb from the initial moisture content to 51% MC, the end of the first step. Actually, this was certainly not the case but in effect we are treating an entire kiln charge as a single sample (and a single moisture profile) so any drop in dry bulb temperature across the charge during the early stages of drying will result in lower drying rates than would result from a small specimen. But this does serve to illustrate both the strengths and the limits of the single profile program.

For the data in Fig. 1 (and using arbitrarily assumed density and half-thickness values),

$$QRATES = \left(\frac{\Delta MC \%}{\Delta Time}\right)\left(\frac{density \times half\text{-}thickness}{100\% \times W.B. \text{ dep.}}\right)$$

$$= \left(\frac{81\% - 51\%}{7.2 \text{ days}}\right)\left(\frac{.58 \text{ g} \times 1.3 \text{ cm}}{100\% \times \text{cm}^3 \times 4 \text{ F}}\right) = 0.7854 \times 10^{-2}\frac{g}{\text{cm}^2\text{day}°\text{F}}$$

If the first listed step of the kiln schedule does not accommodate the input data (e.g., suppose the initial MC were 41%), then the steps will be skipped in sequence until the correct starting step is reached (step #3 for a 41% initial MC). If, through some error in defining the data, all steps are skipped, then the error message "SORPTION SCHEDULE DOES NOT ACCOMMODATE THE INPUT DATA" will be printed to identify the cause of the failure. The computer traverses the steps sequentially so once a step is passed, it cannot be recalled. Thus if an initial MC of 41% and initial temperature, TW, of only 30 F were used, step #2 would be bypassed (41.3% > 41.0%) and the run would start in step #3. But condensation (adsorption) on the cold wood will soon raise its moisture content above 41.3%. Nevertheless, the program will stay in step #3 until the wood dries to below 34.5%.

The NSD(I) = 0 code results in complete blockage of vapor transfer at the air-wood interface, although interface heat transfer, as well as moisture diffusion in the wood profile, continues. If continued long enough, the wood temperature, TW, will virtually reach the ambient air temperature, TDB, and the moisture profile will level out (even if above fiber saturation, which is probably undesirable). In
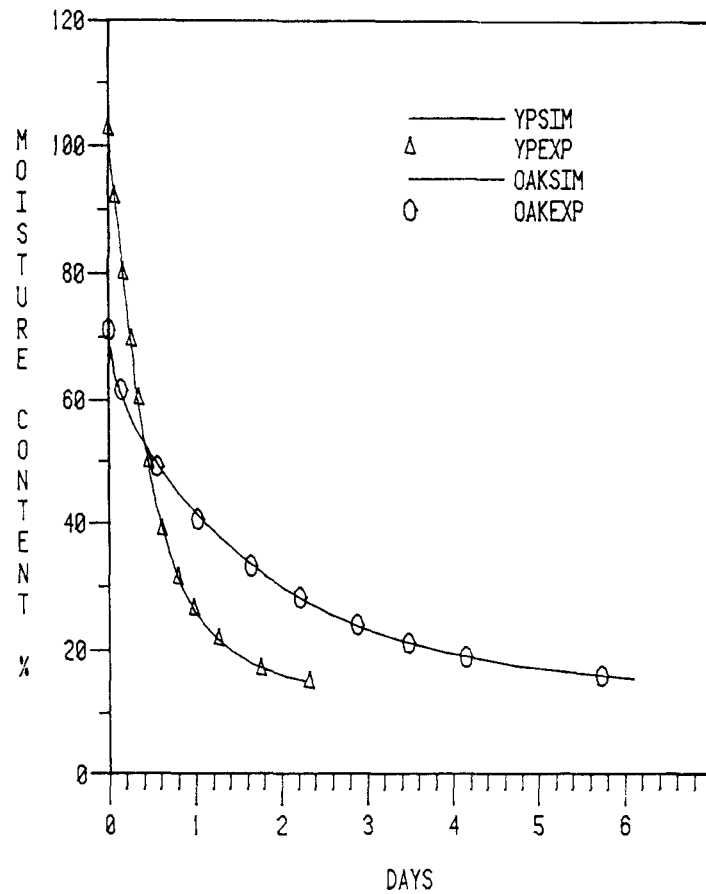
FIG. 3.   Simulated curves fitted to both yellow poplar and white oak experimental data from the same drying conditions.

effect, for a very tight kiln, this simulates closing the vents and turning off the steam spray but keeping the fans on and the heating coils operating. However, it does not simulate board to board exchanges since only a single profile is included.

SIMSOR is programmed to print out not only at the intervals specified by WRT but also at the start of drying and just before each step change. Thus if WRT is in % MC (IWRT = 1) and is sufficiently large (larger than the moisture content change that occurs during the step), print-out would not occur during a step but only at the change to the next step. The print-out data would then summarize the results for the entire step. Additional step cards which duplicate the existing step cards except for different TEST values may be inserted to obtain print-out at specifically desired moisture contents or at desired time intervals, thus giving print-outs to closely match experimental data levels if desired.

Card 8A . . . The final data cards define the initial moisture content profile. Seven values may be put on each card, but if a uniform (flat) profile is desired,

then only the first value on the first card need be entered since it will be duplicated for all N cells. However, any shape of initial profile can be obtained by listing the desired moisture content of each cell. If the total number listed is less than the number of cells, N, as defined in card #2, then the last value before the zero or blank will be replicated to obtain N values. This moisture content listing must end with a blank card to notify the computer to stop reading.

The card following this blank moisture content card is read as the ID of the next data set. A blank card here signifies that no data set follows. Any number of data sets can be entered but the last one must be followed by a blank card for the next ID card (in addition to the blank card for terminating the moisture content reading).

Print Output. The print-out from SIMSOR first lists the input data just as shown in Table 1. It then lists the average moisture content, CBARP, and F(I) for 0.0 to 210% MC at MC intervals of 2.5%. This completes the input data page.

The output data begins with the ID and DESCR(I) on line #1, then on line #3 the labels for the step data in the order of NSD, TEST, QRATES, T$Q, RDB (relative vapor pressure of the air), NS (the step number), EMC, TDB, TWB, and, to the far right, J (the total number of main loops) and NPL (the number of profile loops in the last main loop). These labels are printed only once but the variables will be printed at the start of each step.

Line #5 consists of the following labels.

% CBARP	C-BAR-PROFILE, the current average moisture content of the profile
TIME	Current time
% CBARAV	C-BAR-AVERAGE, average MC for the print-out interval
AVRATE %/T	Average rate of drying for the print-out interval (% MC/time)
TW	Current wood temperature (°F)
RW	Current relative vapor pressure of the wood surface (C(1))
K	Total number of print-out intervals plus one
DELTEF	DELT efficiency, a measure of the operating efficiency.

The ten % MC values for the cells specified by NCLM(I) complete the output. With the input data listed in Table 1, SIMSOR will print out all of the data listed in line #5 for every 1% MC change (since WRT = 1). It will end with 8.84% MC in 22.94 days for % CBARP and TIME. The program listing in the appendix is complete except for the data cards in Table 1 and the necessary job control cards.

This completes the basic information required for the use of SIMSOR. While the input data are somewhat lengthy, it does permit substantial flexibility in the application of the program. Except for defining D$T and its variation with moisture content, none of the other parameters should pose any problem. And the only problem with the diffusion coefficient arises when one is trying to fit the simulation to experimental data.

INPUT DATA LIMITATIONS

There are some limitations on the input data for SIMSOR. As already indicated, the wood temperature, TW, must be less than 250 F and greater than 0 F to

satisfy the present requirements of the isotherm. But since neither boiling nor freezing are dealt with in the program, SIMSOR is technically applicable within 32 to 212 F only. The wet bulb temperature must be less than the dry bulb temperature but a 0.01 F difference (probably even less) is acceptable. In calculating a relative vapor pressure to match the surface MC of the wood, the computed value, which must be less than unity, will not exceed $1.0 - 1.0 \times 10^{-50}$ nor fall below a 0.01 value. The surface MC will not fall below 0.01% MC.

All combinations of parameters do not run with equal efficiency. High levels of QRATES coupled to low levels of D$T (after temperature adjustment) increase the required computer time, as do low levels of QRATES coupled with high levels of D$T. Thus QRATES levels should not be extended too far beyond realistic values (see Eq. 1). Except for the D$T vs. QRATES interactions, SIMSOR functions with equal efficiency with either uniformly high or low D$T levels since the elapsed simulated time per loop is inversely proportional to the temperature adjusted D$T. However, D$T constant with moisture content is more efficient than is a variable relationship since the highest level controls the time per loop.

COMPROMISES

In a computer simulation of unsteady state moisture diffusion, conditions are held constant all across the profile while the flux rates between all adjacent cells are calculated. These are actually steady-state rates. Then the cells are adjusted to their new values and the process is repeated. There are inherent mathematical limitations on the elapsed simulated time for these steady-state steps. If this elapsed time exceeds a critical level, oscillations or gyrations will set in and the program will mathematically self-destruct when the oscillations result in numbers exceeding the capacity of the computer. But the smaller the time per loop or iteration, the greater the number of loops required, and the greater the cost of running the program.

One compromise that was necessary to obtain a reasonable balance between realism and cost was that a uniform temperature across the wood be adopted. It seems highly probable that this is a necessary compromise. The maximum permissible elapsed time (simulated) per loop is inversely proportional to the diffusion coefficient. Since the diffusion coefficient for heat in wood is hundreds of times larger than typical moisture values, then a variable heat profile should increase the cost by the same order of magnitude. It may be possible to use far fewer cells for a temperature profile (compared with a separate moisture profile in the same program) and use many loops across the temperature profile for each loop across the moisture profile, but it doesn't look too promising. Even in SIMSOR, with its uniform temperature profile, the cost of the temperature transfer limitation is not minimal. It was necessary to provide a mechanism for reducing the moisture-dependent maximum permissible loop time (DELT) to the temperature-dependent maximum permissible time (DELTP) whenever required. The recognition of and the solution of this problem was by far the major obstacle encountered in the development of this simulation.

A second compromise proved necessary in equating the diffusion transfer to the vapor transfer at the surface. The approach adopted herein was to calculate the magnitude of the surface transfer (SORATE), based upon the vapor pressure
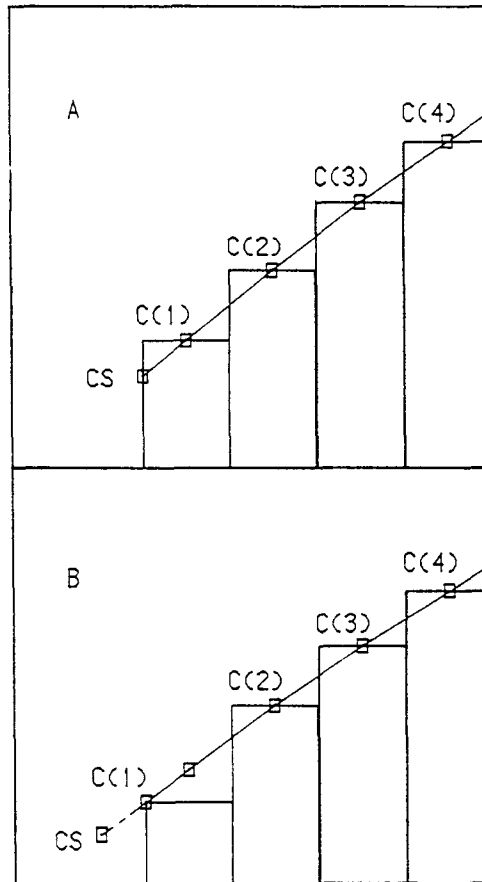
FIG. 4. The optimum treatment of the profile surface is shown in (A), but the compromise treatment that proved necessary for the dummy variable, CS, and the first profile cell, C(1), is shown in (B).

difference between the wood and the air, and then to require an equal rate of diffusion between the first cell, C(1), and CS, a dummy variable. Since CS is a dummy variable, it is not included as part of the actual profile so any transfer to it changes the amount of moisture in the wood. Thus, it is only necessary to set CS to whatever value will cause this diffusion transfer to exactly equal the vapor transfer.

The ideal solution, as shown in Fig. 4A, is to have CS be the wood surface moisture content, even though it is still a dummy variable and thus excluded when the cells are averaged to determine the average moisture content. In this case,

(1) vapor transfer is proportional to the vapor pressure difference between the air and CS, and

(2) diffusion transfer is proportional to the moisture content difference between CS and C(1) (with due account taken for the diffusion coefficient), which are separated by a distance of 0.5 (A/N) cm.

This required seeking a value for CS that would make the vapor transfer in (1) equal the diffusion transfer in (2). Not only did this require an iterative solution, but also it did not prove workable under all of the conditions desired for a widely applicable program. Thus it proved necessary to alter (1) by setting the vapor transfer proportional to the vapor pressure difference between the air and C(1), rather than CS. The required value of CS to satisfy (2) is thus readily determinable without iteration. However, this resulted in the initial sorption rates being excessively rapid. This inaccuracy was largely corrected by considering the moisture in C(1) to be located at the cell surface (Fig. 4B) rather than at the cell center, as is the case with all other cells. This is accomplished very simply by introducing the term SC (= 2/3) into the profile calculations. Its magnitude results from the fact that the C(1) moisture is now 50% further from the C(2) moisture than is the distance (A/N) between the centers of all of the remaining cells. The slope of the moisture profile at the surface is then quite correct, but the moisture content of the C(1) cell is inaccurate. However, with thirty cells, this inaccuracy is of very minor importance except when the surface slope is extremely steep. But to some extent, this steepness accompanies any change in environment. For improved accuracy in the first few loops, N can also be increased, but the computing cost will rise.

If desired, Fickian diffusion at constant temperature and surface moisture content can be very precisely simulated with three internal program alterations, namely, by setting SC = 1, TW = TDB and CS = EMC. This output can then be compared with the normal program employing a high QRATE value relative to D$T (temperature adjusted), which should then closely approximate Fickian diffusion since the surface will quickly approach EMC. For any fraction of total drying, the normal program time will be within 1% of the Fickian time except during the very early loops when the surface profile is first being established.

The two parameter relative vapor pressure vs. equilibrium moisture content isotherm employed in SIMSOR is a compromise in the sense that it is asymptotic to RVP = 1. This simplifies the unified treatment of free and bound water. The ambient EMC actually plays no role in the SIMSOR program other than as a reference point for terminating the run. Thus if the EMC were 40% and the wood moisture content were 30%, virtually no sorption would occur because of the very small difference in vapor pressure, which is what controls the surface transfer. This makes it possible for the program to deal effectively and realistically with humidities approaching 100%, which is essential for duplication of air drying. Another attribute of the isotherm is the ease of defining it with only two experimental pairs of RVP-EMC data points. Also, for future development, the isotherm differential can be employed as a multiplier in the profile to convert from moisture content difference to vapor pressure difference as the basis for moisture transfer, as employed by Bramhall (1979). If coupled with a temperature profile, this may permit a realistic simulation of hydrodynamic flow in high temperature drying, but would seem to offer little advantage for temperatures below the boiling point.

The last compromise is in the treatment of the free water. In this program, the free water is treated exactly the same as the bound water, that is, as a diffusion phenomenon dependent upon the moisture difference between cells, the diffusion coefficient and the saturated vapor pressure. However, free water flow is a capillary flow phenomenon rather than a diffusion phenomenon and presumably should not be as vapor pressure dependent as bound water diffusion is, so a change in drying temperature should affect the free water flow rate much less than it affects the bound water rate. Thus, by adjusting their relative diffusion coefficients to their 80 F values (an arbitrary level), the vapor pressure adjustment can be canceled for all cells whose moisture contents exceed TDL. However, it is possible that free water flow is almost totally a function of the particular anatomical arrangement of the inter-connecting capillaries coupled with the below fiber saturation rate of transport. *Thus the relative shapes of the bound water versus free water portions of the moisture profile could be quite independent of the temperature at which the wood is dried.* If this proves true, then TDL should be set beyond the maximum moisture content so that the free water will be treated just as is the bound water. This was done in the examples given herein. In summary, free water is treated as bound water in this program but its temperature dependence may be canceled, if desired. Whether or not this will provide adequately for the free water flow remains to be determined, but it does provide for flexibility in the early applications of this program.

PROGRAMMING CONSIDERATIONS

From QRATES, the surface transfer coefficient, two related coefficients are derived in the program. The first is the vapor transfer coefficient, QRAT$P (g cm $^{-2}$ time^{-1} psi^{-1}), which is obtained from division of QRATES by (B*APT$Q), the product of the barometric pressure, B (psi), and the psychrometric constant, AP, at temperature T$Q, hence, APT$Q (1/°F). The second is the heat transfer coefficient (cal. cm^{-2} time^{-1} °F^{-1}), which is obtained from multiplication of QRATES by (APTW/APT$Q)*(HTLAT) (the psychrometric constant ratio times the latent heat) but which does not have an assigned variable name for the sake of computing efficiency. Both of these surface transfer coefficients, vapor and heat, are temperature-independent so vapor transfer is always proportional to the vapor pressure difference while heat transfer is proportional to the temperature difference, regardless of the levels of temperature involved. The temperature-dependent psychrometric constant is from the Smithsonian Tables (see Bindon 1963). The latent heat is also temperature-dependent (Weast 1973). Their product is constant with temperature (variable latent heat is the reason for the temperature dependency of the psychrometric constant—hence, the constant product of the two). Both the vapor and the heat transfer coefficients are assumed to hold constant throughout the sorption run, unless the air velocity is altered.

Most of the variables in SIMSOR are dependent on either the wood temperature or moisture. Those that are neither are computed either before the main loop (JJ loop) or in the Sorption Schedule Step Selection routine at the beginning of the main loop. As previously indicated, there is a moisture-dependent maximum elapsed time, DELT, and a separate heat controlled value, DELTP. The smaller of the two is used for the profile loop, that is, for the loop in which the cell-to-

cell changes in the profile are calculated. DELT is used in the outer loop, and the inner or profile loop is repeated as many times as necessary to insure that the time per profile loop does not exceed DELTP. Thus, for each passage through the outer loop, this iteration of the profile may vary from one to several hundred loops, depending on the input data. The less sensitive temperature- or moisture-dependent variables are computed prior to the profile loop. Only the most critical variables are always computed for each passage across the profile loop. The less sensitive variables include the isotherm variables (BCS and QCS), the diffusion coefficient's moisture content dependency (F(I)), latent heat (HTLAT), relative differential heat (DIFHT), heat capacity (CD), psychrometric constant (APTW), heat transfer coefficient (from QRATES), and a REDFAC routine which, if necessary, will reduce the time interval (DELT) to a value that insures that the subsequent change in the wood temperature (TW) will not exceed the value TWDLT specified by the input data. Next comes the Profile routine, which is the heart of the simulation.

The Profile routine handles all changes in the wood moisture contents, relative vapor pressure, actual vapor pressure and temperature. The rationale and order of computation are as follows. Given the surface moisture content (C(1)), RFI (i.e., 1 − relative vapor pressure) is calculated from the moisture content vs. relative humidity isotherm. The relative humidity times the saturated vapor pressure (PWP) at the wood temperature (TW) gives the vapor pressure of the wood surface. With this vapor pressure, the partial vapor pressure of the air, and the vapor transfer coefficient (QRAT$P, previously calculated in the Sorption Schedule Step Selection routine), the vapor transfer rate (SORATE) between the air and the wood is obtained. Next the value of the dummy variable (CS), necessary to make the diffusion transfer equal the vapor transfer, is determined. The profile is then traversed, after which the new values for C(I) are adopted. Finally, the new wood temperature (TW) and saturated vapor pressure (PWP) are calculated. The wood temperature results from three sources: the heat exchanged between the air and the wood, the latent heat plus differential heat involved in the change in state between water and vapor, and the sensible heat involved in any change in the wood temperature.

In all of these Profile routine calculations, unnecessary repetitions are avoided by putting all possible portions of each calculation above the profile loop. The most intricate example of this is probably in the moisture flux calculations. The moisture content of each profile cell changes according to the balance between the inflow and outflow from and to the adjacent cells. Taking just one of these flux terms,

$$. . . V^*(F(I)^*(C(I - 1) - C(I)) . . .)$$

the fundamental character can be determined by tracing the path of V back up through the program and substituting the indicated variables into the flux expression.

$$DELT^*(D\$T^*(PWP/PT\$D)^*F(I))^*(C(I - 1) - C(I))/(A/N)^{**}2$$

will be obtained from these substitutions. This is the steady-state flux in % MC that results from the products of time (DELT), unsteady-state diffusion coefficient

(D$T), corrected for temperature by the saturated vapor pressure ratio (PWP/PT$D) and for moisture content by F(I), with the final term being the slope or moisture gradient, which is the moisture difference (C(I − 1) − C(I)) divided by the distance between the cells (A/N). The between cell distance is equal to the cell thickness, which is also involved for the conversions between steady and unsteady-state diffusion coefficients and in obtaining the flux in % MC rather than in weight of water, so (A/N) appears as a squared term. In this manner, the multiplier V*F(I) is kept as close to the critical value of 0.5 as deemed advisable and DELT is varied directly with the square of the cell thickness and inversely with the temperature corrected diffusion coefficient.

While the critical level for stability, 0.5, for the moisture profile multiplier can be mathematically demonstrated, the rationale for the manner in which heat transfer controls the maximum permissible time interval, DELTP$, was not precisely defined. The DELTP$ equation at the start of the Profile routine is an empirical equation based upon trial and error. The critical level of DELTP$ was clearly a function of SG, A, QRATE and PW (the rest were judgment values), but the level varied with different combinations of wood moisture and drying conditions in a manner that could not be precisely defined. The constant of 60 was very extensively tested and is believed to be safe for all conditions between 0 and 250 F, but a lower value would be more economical and many typical trials worked perfectly with a value of 20. As a precautionary measure, the print-out variable, DELTEF (DELT efficiency), is included to indicate when the time (DELT) per main loop has been reduced, either by the REDFAC routine or near the end of the Profile routine, to prevent the change in TW from exceeding TWDLT. This occurs naturally when environmental conditions are changed but under stable conditions, DELTEF should remain at 100. If oscillations do occur, it should be apparent.

VERIFICATION

SIMSOR has been tested sufficiently to make it virtually certain that it will properly function in the mathematical sense with any realistic combination of input variables that might be employed. It now must be tested against the widest possible range of experimental data. It will readily simulate small specimens exposed to a single drying atmosphere, as illustrated in Fig. 3. It has also accurately duplicated similar specimens exposed to a 24-hour sinusoidal temperature and has even duplicated with excellent accuracy the drying behavior of red oak sandwiched between plywood panels to protect the wood from excessively rapid drying (Schultz 1978). Figure 1 shows that it can satisfactorily simulate a kiln schedule. But in all of these applications, the diffusion coefficient could be varied to suit the particular sample. What is now needed are data from carefully matched specimens, with adequate replication, exposed to a variety of environmental conditions. This can be most quickly accomplished by a variety of investigators who have need for a simulation and have data to be evaluated. Of particular need are data on matched green specimens dried at different temperature levels to assess the effect of temperature on the relative behavior of free water versus bound water. And this is needed for a variety of species, both softwood and hardwood, so the task is sizable.

Even at the present level of verification, SIMSOR can provide very useful estimates. Only long-term verification will determine the final accuracy. In any event, it will be a valuable tool for drying research. Since it is based upon clearly defined and specified principles, it can serve as a reference standard against which the observed behavior of actual data can be judged and interpreted.

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Note: Upon request, the author will provide a tape of the program at cost.

APPENDIX

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C - - SIMSOR: A COMPUTER SIMULATION OF WATER SORPTION IN WOOD (IN         1
C - - FORTRAN IV) BY C. ARTHUR HART, SCHOOL OF FOREST RESOURCES,          2
C - - NORTH CAROLINA STATE UNIVERSITY, RALEIGH, N.C. 27650                3
      IMPLICIT REAL*8(A-H,O-Z)                                           4
      DIMENSION C(112),CA(110),CB(110),F(110),CMP(110)                   5
      DIMENSION DESCR(70),NCLM(10),CWRITE(10)                            6
      DIMENSION TDBS(99),TWBS(99),TEST(99),NSD(99),QRATES(99),TSQS(99)   7
      ABS(X)=DABS(X)                                                     8
      EXP(X)=DEXP(X)                                                     9
      ALOG(X)=DLOG(X)                                                    10
      SIN(X)=DSIN(X)                                                     11
      CALL ERRSET(208,256,-1,1,0,0)                                      12
C                                                                        13
C - - D=DIFFUSION COEFFICIENT, A=HALF THICKNESS, N=NO. OF CELLS IN THE    14
C - - PROFILE, DELT = ELAPSED TIME PER PROFILE LOOP. DELT MUST BE LESS    15
C - - THAN (0.5*(A/N)**2)/D & SHOULD NOT EXCEED 0.4*(A/N)**2/D. THIS      16
C - - GIVES V = 0.4 WHERE V = (DELT * D)/((A/N)**2                        17
C                                                                        18
C                                                                        19
    5 READ (1,15) ID,(DESCR(I),I=1,69)                                   20
   15 FORMAT (I10,1X,69A1)                                               21
      IF (ID) 885,885,25                                                 22
   25 CONTINUE                                                           23
      READ (1,35) SG,A,N,TW,TWDLT,TDL                                    24
   35 FORMAT (10X,2(1X,F9.3),8X,I2,3(1X,F9.3))                           25
      READ (1,45) DST,TSD,BWDM,CBWDM,RBWDM                               26
   45 FORMAT (11X,E9.4,5(1X,F9.3))                                       27
      READ (1,55) FWL,FWDBL,FWDM,CFWDM,RFWDM                             28
   55 FORMAT (10X,7(1X,F9.3))                                            29
      READ (1,65) RVPSH,EMCSH,RVPSL,EMCSL,TSEMC,B                        30
   65 FORMAT (10X,6(1X,F9.4))                                            31
      READ (1,75) IWRT,WRT,FINIS,JJ,(NCLM(I),I=1,10)                     32
   75 FORMAT (19X,I1,2(1X,F9.3),1X,I9,10X,10I2)                          33
      WRITE (3,85)                                                       34
   85 FORMAT (1H1)                                                       35
      WRITE (3,95)                                                       36
   95 FORMAT (1H0,8X,'ID',10X,'DESCR(I)')                                37
      WRITE (3,105) ID,(DESCR(I),I=1,69)                                 38
  105 FORMAT (1H ,I10,1X,69A1)                                           39
      WRITE (3,115)                                                      40
  115 FORMAT (1H0,T20,'SG',T31,'A',T41,'N',T50,'TW',T57,'TWDLT',T69,'TDL 41
     1')                                                                 42
      WRITE (3,125) SG,A,N,TW,TWDLT,TDL                                  43
  125 FORMAT (1H ,10X,2(1X,F9.5),8X,I2,3(1X,F9.5))                       44
      WRITE (3,135)                                                      45
  135 FORMAT (1H0,T19,'DST',T29,'TSD',T38,'BWDM',T47,'CBWDM',T57,'RBWDM' 46
     1)                                                                  47
      WRITE (3,145) DST,TSD,BWDM,CBWDM,RBWDM                             48
  145 FORMAT (1H ,11X,E9.4,5(1X,F9.5))                                   49
      WRITE (3,155)                                                      50
  155 FORMAT (1H0,T19,'FWL',T27,'FWDBL',T38,'FWDM',T47,'CFWDM',T57,'RFWD 51
     1M')                                                                52
      WRITE (3,165) FWL,FWDBL,FWDM,CFWDM,RFWDM                           53
  165 FORMAT (1H ,10X,7(1X,F9.5))                                        54
      WRITE (3,175)                                                      55
  175 FORMAT (1H0,T17,'RVPSH',T27 'EMCSH',T37,'RVPSL',T47,'EMCSL',T57,'T 56
     1SEMC',T71,'B')                                                     57
      WRITE (3,185) RVPSH,EMCSH,RVPSL,EMCSL,TSEMC,B                      58
  185 FORMAT (1H ,10X,6(1X,F9.5))                                        59
      WRITE (3,195)                                                      60
```

APPENDIX

```
 195 FORMAT (1H0,T18,'IWRT',T29,'WRT'T37,'FINIS',T50,'JJ',T68,'NCLM(I)'     61
    1)                                                                        62
     WRITE (3,205) IWRT,WRT,FINIS,JJ,(NCLM(I),I=1,10)                         63
 205 FORMAT (1H ,19X,I1,2(1X,F9.5),1X,I9,10X,10I2)                            64
     WRITE (3,215)                                                            65
 215 FORMAT (1H0,T15,'TDBS(I)',T25,'TWBS(I)',T36,'NSD(I)',T45,'TEST(I)'       66
    1,T53,'QRATES(I)',T65,'TSQS(I)')                                          67
     QR=0.0                                                                   68
     TQ=0.0                                                                   69
     DO 245 I=1,99                                                            70
     READ (1,225) TDBS(I),TWBS(I),NSD(I),TEST(I),QRATES(I),TSQS(I)           71
 225 FORMAT (10X,2(1X,F9.4),8X,I2,1X,F9.4,1X,E9.4,1X,F9.4)                    72
     IF (QRATES(I).EQ.0.0)QRATES(I)=QR                                        73
     IF (TSQS(I).EQ.0.0)TSQS(I)=TQ                                            74
     QR=QRATES(I)                                                             75
     TQ=TSQS(I)                                                               76
     WRITE (3,235) TDBS(I),TWBS(I),NSD(I),TEST(I),QRATES(I),TSQS(I)          77
 235 FORMAT (1H ,10X,2(1X,F9.4),8X,I2,1X,F9.4,1X,E9.4,1X,F9.4)               78
     IF (TDBS(I)) 255,255,245                                                 79
 245 NSMX=I                                                                   80
 255 CONTINUE                                                                 81
     WRITE (3,265)                                                            82
 265 FORMAT (1H0,10X,7(6X,'C(J)'))                                            83
     DO 275 I=1,N                                                             84
 275 C(I)=0.0                                                                 85
     N1=1                                                                     86
     N2=7                                                                     87
     DO 305 I=1,16                                                            88
     READ (1,285) (C(J),J=N1,N2)                                             89
 285 FORMAT (10X,7(1X,F9.4))                                                  90
     IF (C(N1).LE.0.0) GO TO 315                                              91
     WRITE (3,295) (C(J),J=N1,N2)                                             92
 295 FORMAT (1H ,10X,7(1X,F9.4))                                             93
     N1=N1+7                                                                  94
 305 N2=N2+7                                                                  95
 315 SUMC=C(1)                                                                96
     DO 325 I=2,N                                                             97
     IF (C(I).LE.0.0)C(I)=C(I-1)                                              98
 325 SUMC=SUMC+C(I)                                                           99
     CBARP2=SUMC/N                                                           100
     CBARP=CBARP2                                                            101
     WRITE (3,335)                                                           102
     WRITE (3,345)                                                           103
     WRITE (3,355) CBARP2                                                    104
 335 FORMAT (1H0,10X,'THE FOLLOWING ARE CALCULATED DATA')                   105
 345 FORMAT (1H0,T11,'CBARP')                                               106
 355 FORMAT (1H ,T10,F6.2)                                                   107
C                                                                           108
C - - START CALCULATION OF DIFFUSION COEFFICIENT'S MC DEPENDENCY.          109
     BWLC=CBWDM-RBWDM/2.                                                    110
     BWUC=CBWDM+RBWDM/2.                                                    111
     FWLC=CFWDM-PFWDM/2.                                                    112
     FWUC=CFWDM+RFWDM/2.                                                    113
     CM=-2.5                                                                114
     DO 385 I=1,85                                                          115
     CM=CM+2.5                                                              116
     CMP(I)=CM                                                              117
     IF (CMP(I).GT.FWL) GO TO 365                                           118
     F(I)=1.                                                                119
     IF (CMP(I).GT.BWLC.AND.CMP(I).LT.BWUC)F(I)=1.+(BWDM-1.)*0.5*(1.+SI    120
    1N(3.14*(CMP(I)-CBWDM)/RBWDM))                                         121
     IF (CMP(I).GE.BWUC)F(I)=BWDM                                          122
     GO TO 375                                                             123
 365 F(I)=FWDBL                                                             124
     IF (CMP(I).GT.FWLC.AND.CMP(I).LT.FWUC)F(I)=FWDBL+(FWDM-FWDBL)*0.5*    125
    1(1.+SIN(3.14*(CMP(I)-CFWDM)/RFWDM))                                   126
     IF (CMP(I).GE.FWUC)F(I)=FWDM                                          127
 375 CONTINUE                                                               128
 385 CONTINUE                                                               129
     IS=1                                                                   130
```

```
      IE=17                                                              131
      DO 435 IL=1,5                                                     132
      WRITE (3,395)                                                     133
395 FORMAT (1H0,3X,'%MC=')                                             134
      WRITE (3,405) (CMP(I),I=IS,IE)                                   135
405 FORMAT (1H+,7X,17(2X,F5.1))                                       136
      WRITE (3,415)                                                     137
415 FORMAT (1H ,2X,'F(I)=')                                           138
      WRITE (3,425) (F(I),I=IS,IE)                                     139
425 FORMAT (1H+,7X,17(1X,F6.3))                                       140
      IS=IS+17                                                          141
435 IE=IE+17                                                           142
C - - END CALCULATION OF DIFFUSION COEFFICIENT'S MC DEPENDENCY.        143
C                                                                       144
      WRITE (3,445) ID,(DESCR(I),I=1,69)                              145
445 FORMAT (1H1,7X,I10,4X,69A1)                                       146
      WRITE (3,455)                                                     147
455 FORMAT (1H0,T6,'NSD',T16,'TEST',T33,'QRATES',T43,'T$Q',T49,'RDB',T 148
     154,'NS',T67,'%EMC',T75,'TDB',T82,'TWB',T126,'J',T131,'NPL')     149
      WRITE (3,465)                                                     150
465 FORMAT (T1,'0',T3,'%CBARP',T16,'TIME',T21,'%CBARAV',T29,'AVRATE %/ 151
     1T',T44,'TW',T50,'RW',T55,'K',T58,'DELTEF',T65,'S')              152
      WRITE (3,475) (NCLM(I),I=1,10)                                   153
475 FORMAT (T1,'+',T64,10(2X,'%MC',I2))                              154
      WRITE (3,485)                                                     155
485 FORMAT (T1,' ')                                                    156
C                                                                       157
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -   158
C                                                                       159
      AVRATE=0.0                                                       160
      CBARAV=CBARP2                                                    161
      DELT8S=0.0                                                       162
      K=1                                                              163
      LL=N-1                                                           164
      NPL=1                                                            165
      NS=0                                                             166
      REDFAC=1.                                                        167
      SC=2./3.                                                         168
      TIMEK=0.0                                                        169
      TIMET=0.                                                         170
      TST=0.0                                                          171
      WTCHNG=0.0                                                       172
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -   173
C                                                                       174
C + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +   175
      T1=T$D                                                           176
      NOSTA=3                                                          177
      GO TO 505                                                        178
495 PT$D=P2                                                            179
      DX$=D$T/(A/N)**2                                                180
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - -          181
      GO TO 515                                                        182
505 T2=273.+(T1-32.)/1.8                                             183
      P2=EXP(14.375309-3736.763/T2-(481.7725/T2)**2)                 184
C - - P2 ( IN PSI ) IS THE SATURATED VAPOR PRESSURE OF WATER AT TEMP T2. 185
      GO TO (615,625,495,675),NOSTA                                  186
515 CONTINUE                                                          187
C                                                                       188
C-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-      189
C                                                                       190
C - - CALCULATE THE EMC-RH ISOTHERM PARAMETERS.                        191
      TOP=ALOG(EMC$H)-ALOG(EMC$L)                                      192
      BOT=ALOG(-ALOG(1.-RVP$H))-ALOG(-ALOG(1.-RVP$L))                  193
      Q$CS=TOP/BOT                                                     194
      B$CS=EMC$L/(-ALOG(1.-RVP$L))**Q$CS                             195
C                                                                       196
      BBAS=12.25-6.2488*(1.-EXP(-(T$EMC/170.)**2.9038))              197
C - - T$EMC .GT. 0. BUT SHOULD BE WITHIN 32 TO 212 FOR BBAS            198
      QBAS=0.61+0.1078*(-ALOG(1.-T$EMC/250.))**0.8467                199
C - - 0. .LT. T$EMC .LT. 250. BUT SHOULD BE WITHIN 32 TO 212 FOR QBAS 200
```

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C                                                                    201
C                                                                    202
C-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-        203
      DO 845 J=2,JJ                                                  204
C - - THIS IS THE MAIN, OUTER, J OR JJ LOOP.                         205
C-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-        206
C                                                                    207
C - - START OF SORPTION SCHEDULE STEP SELECTION - - - - - - - - - -  208
      IF (NS.NE.0) GO TO 565                                         209
C - - NS=0 ROUTINE TO SELECT THE PROPER FIRST SORPTION SCHEDULE STEP. 210
  525 NS=NS+1                                                        211
      IF (NS.LE.NSMX) GO TO 545                                      212
      WRITE (3,535)                                                  213
  535 FORMAT (T1,'0',T2,'SORPTION SCHEDULE DOES NOT ACCOMODATE THE INPUT 214
     1 DATA.')                                                       215
      GO TO 855                                                      216
  545 CONTINUE                                                       217
      IF (NSD(NS).EQ.2.OR.NSD(NS).EQ.0) GO TO 605                    218
      IF (NSD(NS).EQ.1) GO TO 555                                    219
      IF (CBARP.LT.TEST(NS)) GO TO 525                               220
      GO TO 605                                                      221
  555 IF (CBARP.GT.TEST(NS)) GO TO 525                               222
      GO TO 605                                                      223
C - - END OF NS=0 ROUTINE - - - - - - - - - - - - - - - - - - - - -  224
  565 CONTINUE                                                       225
      IF (NSD(NS).EQ.1) GO TO 575                                    226
      IF (NSD(NS).EQ.2.OR.NSD(NS).EQ.0) GO TO 585                    227
      IF (CBARP.LT.TEST(NS)) GO TO 595                               228
      GO TO 665                                                      229
  575 IF (CBARP.GT.TEST(NS)) GO TO 595                               230
      GO TO 665                                                      231
  585 IF (TIMET.GE.TEST(NS)) GO TO 595                               232
      GO TO 665                                                      233
C                                                                    234
C + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +    235
C                                                                    236
  595 IF (TIMET.NE.TIMEK) GO TO 805                                  237
      NS=NS+1                                                        238
  605 CONTINUE                                                       239
      IF (NSD(NS).EQ.2.OR.NSD(NS).EQ.0)TEST(NS)=TEST(NS)+TIMET       240
      IF (NS.GT.NSMX) GO TO 855                                      241
      TDB=TDBS(NS)                                                   242
      TWB=TWBS(NS)                                                   243
      QRATES=QRATES(NS)                                              244
      T$Q=T$QS(NS)                                                   245
C                                                                    246
C-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-        247
C                                                                    248
      T1=TDB                                                         249
      NOSTA=1                                                        250
      GO TO 505                                                      251
  615 PDB=P2                                                         252
      T1=TWB                                                         253
      NOSTA=2                                                        254
      GO TO 505                                                      255
  625 PWB=P2                                                         256
C - - PDP=PWB-0.005374*(TDB-TWB) IF B=14.43(PSI) & APT$Q=3.724E-4(1/F) 257
      APT$Q=(.367E-3)*(1.+(T$Q-32.)/1571.)                          258
C - - APT$Q(1/FAHR)=PSYCHROMETRIC CONSTANT AT TEMPERATURE T$Q       259
      APTWB=(.367E-3)*(1.+(TWB-32.)/1571.)                          260
C - - PSYCHROMETRIC EQUATION IS NEXT. PDP=PRESSURE DEW POINT (PSI).  261
      PDP=PWB-B*APTWB*(TDB-TWB)                                      262
      PDB=PDP/PDB                                                    263
      QRAT$P=QRATES/(B*APT$Q)                                        264
C - - QRAT$P (IN G/SQ CM,TIME,PSI)=VAPOR TRANSFER COEFFICIENT        265
C - - NEXT SET THE ISOTHERM TO THE DRY BULB TEMP, TDB.              266
      BCS=(B$CS/BBAS)*(12.25-6.249*(1.-EXP(-(TDB/170.)**2.8038)))    267
      QCS=(Q$CS/QBAS)*(0.61+0.1078*(-ALOG(1.-TDB/250.))**0.8467)     268
      EMC=BCS*(-ALOG(1.-PDB))**QCS                                   269
C                                                                    270
```

```
      WRITE (3,635) NSD(NS),TEST(NS),QRATE$,T$Q,RDB,NS,EMC,TDB,TWB,J,NPL   271
  635 FORMAT (1H0,I7,1X,F10.2,9X,E10.4,1X,F6.2,1X,F5.3,1X,I3,8X,3(1X,F6.   272
     12),35X,I7,2X,I5/)                                                    273
      IF (J.NE.2) GO TO 665                                               274
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -  275
C                                                                         276
      DO 645 I=1,10                                                       277
      LC=NCLM(I)                                                          278
  645 CWRITE(I)=C(LC)                                                     279
C                                                                         280
      WRITE (3,655) CBARP2,TIMEK,CBARRAV,AVRATE,TW,(CWRITE(I),I=1,10)     281
  655 FORMAT (1H ,1X,F6.2,1X,E10.4,1X,F7.3,1X,E10.4,1X,F6.2,18X,10(1X,F6  282
     1.2))                                                                283
C - - END OF SORPTION SCHEDULE STEP SELECTION - - - - - - - - - - - - -   284
C                                                                         285
  665 CONTINUE                                                            286
C                                                                         287
      TWB=TW                                                              288
C                                                                         289
C - - NEXT SET ISOTHERM TO WOOD TEMPERTURE, TW.                           290
      BCS=(B$CS/BBAS)*(12.25-6.249*(1.-EXP(-(TW/170.)**2.8038)))          291
C-----TW   .GT. 0. BUT IT SHOULD BE WITHIN 32 TO 212 FOR BCS             292
      QCS=(Q$CS/QBAS)*(0.61+0.1078*(-ALOG(1.-TW/250.))**0.8467)          293
C-----0. .LT. TW    .LT. 250. BUT SHOULD BE WITHIN 32 TO 212 FOR QCS     294
C                                                                         295
      T1=TW                                                               296
      NOSTA=4                                                             297
      GO TO 505                                                           298
  675 PW=P2                                                               299
C                                                                         300
C - - START CALCULATION OF DIFFUSION COEFFICIENT'S MC DEPENDENCY.         301
      FMAX=0.0                                                            302
      DO 705 I=1,N                                                        303
      IF (C(I).GT.FWL) GO TO 685                                          304
      F(I)=1.                                                             305
      IF (C(I).GT.BWLC.AND.C(I).LT.BWUC)F(I)=1.+(BWDM-1.)*0.5*(1.+SIN(3.  306
     114*(C(I)-CBWDM)/RBWDM))                                             307
      IF (C(I).GE.BWUC)F(I)=BWDM                                          308
      GO TO 695                                                           309
  685 F(I)=FWDBL                                                          310
      IF (C(I).GT.FWLC.AND.C(I).LT.FWUC)F(I)=FWDBL+(FWDM-FWDBL)*0.5*(1.+  311
     1SIN(3.14*(C(I)-CFWDM)/RFWDM))                                       312
      IF (C(I).GE.FWUC)F(I)=FWDM                                          313
  695 CONTINUE                                                            314
      IF (C(I).GT.TDL)F(I)=F(I)*0.50683/PW                               315
C - - PW=0.50683 WHEN TW=80. SO FOR MC'S ABOVE TDL,  THE DIFF. COEFF.     316
C - - - IS CORRECTED TO IT'S 80 DEGREE VALUE.                            317
      IF (FMAX.LT.F(I))FMAX=F(I)                                          318
  705 CONTINUE                                                            319
C - - END CALCULATION OF DIFFUSION COEFFICIENT'S MC DEPENDENCY.          320
C                                                                         321
      DO 715 I=1,N                                                        322
  715 CA(I)=C(I)                                                          323
C                                                                         324
      V=0.4/FMAX                                                          325
      DX=DX$*PW/PT$D                                                      326
C - - DIFFUSION COEFFICIENT IS NOW CORRECTED FOR TEMPERATURE, TW          327
      DELT=V/DX                                                           328
C - - DELT=PERMISSABLE TIME PER LOOP FOR MOISTURE DIFFUSION              329
      DELT8=DELT                                                          330
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -  331
      HTLAT=604.19-0.2686*TW-0.00019*TW**2                               332
C - - HTLAT(IN CALORIES/G)=LATENT HEAT AT TEMPERATURE TW.                333
      DIFHT=1.+0.488*EXP(-0.1466*CBARP)                                  334
C - - DIFHT(DIMENSIONLESS)=RELATIVE DIFFERENTIAL HEAT.                   335
      CD=0.266+0.000644*(TW-32.)                                         336
C - - CD(IN CALORIES/G,CELSIUS) = COEFFICIENT OF HEAT CAPACITY. TW(FAHR) 337
      APTW=(.367E-3)*(1.+(TW-32.)/1571.)                                 338
      QRATE=QRATE$*APTW/APT$Q                                            339
C - - QRATE(G/SQ CM, TIME, FAHR)=SURFACE TRANSFER COEFFICIENT AT TEMP TW 340
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C - - QRATE*HTLAT(IN CAL/SQ CM, TIME, F)=HEAT TRANSFER COEFFICIENT. IT      341
C - - IS CONSTANT FOR ALL TW.                                              342
C                                                                          343
C-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+--          344
C                                                                          345
C - - REDFAC ROUTINE TO LIMIT TW CHANGE BY LIMITING DELT - - - - - - -     346
C                                                                          347
      RF1=EXP(-(C(1)/BCS)**(1./QCS))                                       348
C - - RF1(DIMENSIONLESS)=1.-RW WHERE RW=R.V.P. OF THE WOOD SURFACE.        349
      IF (RF1.GT.0.99)RF1=0.99                                            350
      IF (RF1.LT.1.0E-50)RF1=1.0E-50                                      351
      SDRATE=-QRAT$P*(PW-PDP-RF1*PW)                                       352
C - - SDRATE(IN G/SQ CM,TIME)=SURFACE VAPOR TRANSFER RATE.                 353
      IF (NSD(NS).EQ.0)SDRATE=0.0                                         354
      TWUL=DELT*(HTLAT*1.8/((CD+CBARP/100.)*SG*A))                        355
C - - TWUL(IN TIME,FAHR,SQ CM/G)                                          356
      TW2=TW+(QRATE*(TDB-TW)+SDRATE*DIFHT)*TWUL                           357
C                                                                          358
      TWFK=1.                                                             359
      IF (ABS(TW-TW2).LE.TWDLT) GO TO 725                                 360
      TWFK=ABS(TW-TW2)/TWDLT                                              361
  725 CONTINUE                                                            362
C                                                                          363
      REDFAC=1./TWFK                                                      364
      IF (REDFAC.GT.1.0)REDFAC=1.0                                        365
      TW2=TW-(TW-TW2)*REDFAC                                              366
C - - ABS(TW-TW2) IS NOW .LE. TWDLT                                       367
      V=V*REDFAC                                                          368
      DELT=DELT*REDFAC                                                    369
C                                                                          370
C - - END OF REDFAC ROUTINE - - - - - - - - - - - - - - - - - - - - -     371
C                                                                          372
C-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+--          373
C                                                                          374
C - - START OF M.C. PROFILE ROUTINE - - - - - - - - - - - - - - - - -     375
C                                                                          376
C - - NPL=1+60.*.4*PT$D*A*QRATE*HTLAT/(SG*N**2*D$T*FMAX*DIFHT*(CD+CBARP)  377
      DELTP$=SG*A*DIFHT*(CD+CBARP/100.)/(QRATE*HTLAT*PW*60.)              378
C - - DELTP$=PERMISSABLE TIME/LOOP FOR HEAT TRANSFER (EMPIRICAL EQN)       379
      NPL=1+DELT/DELTP$                                                   380
      DELTP=DELT/NPL                                                      381
      V=V/NPL                                                             382
      TWULP=TWUL*DELTP/DELT8                                              383
      SCSPW=-QRAT$P*PW*DELTP*(100.*N/(A*SG*2.*F(1)*V))                    384
C - - SCSPW(IN %) SETS SURFACE DIFFUSION TRANSFER = VAPOR TRANSFER.        385
      PWP=PW                                                              386
      V$=V/PW                                                             387
C                                                                          388
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -       389
      DO 765 IR=1,NPL                                                     390
      V=V$*PWP                                                            391
      RF1=EXP(-(C(1)/BCS)**(1./QCS))                                      392
      SDRATE=-QRAT$P*(PWP-PDP-RF1*PWP)                                    393
      CS=(1.-RF1-PDP/PWP)*SCSPW+C(1)                                      394
C - - THIS SETS THE TRANSFER BETWEEN CS & C(1) EQUAL TO SDRATE.            395
C                                                                          396
      IF (NSD(NS).NE.0) GO TO 735                                         397
      SDRATE=0.0                                                          398
      CS=C(1)                                                             399
  735 CONTINUE                                                            400
C                                                                          401
      CB(1)=C(1)+V*(2.*F(1)*(CS-C(1))-SC*F(2)*(C(1)-C(2)))                402
      CB(2)=C(2)+V*(SC*F(2)*(C(1)-C(2))-F(3)*(C(2)-C(3)))                 403
      DO 745 I=3,LL                                                       404
  745 CB(I)=C(I)+V*(F(I)*(C(I-1)-C(I))-F(I+1)*(C(I)-C(I+1)))              405
      CB(N)=C(N)+F(N)*V*(C(N-1)-C(N))                                     406
      DO 755 I=1,N                                                        407
  755 C(I)=CB(I)                                                          408
C                                                                          409
      TW=TW+(QRATE*(TDB-TW)+SDRATE*DIFHT)*TWULP                           410
```

```
      T2=273.+(TW-32.)/1.8                                              411
      PWP=EXP(14.375309-3736.763/T2-(481.7725/T2)**2)                  412
      IF (C(1).LT.0.01)C(1)=0.01                                       413
      NIR=IR                                                           414
      IF (ABS(TW8-TW).GT.TWDLT) GO TO 775                              415
  765 CONTINUE                                                         416
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -   417
      GO TO 785                                                        418
  775 DELT=DELT*NIR/NPL                                                419
  785 NPL=NIR                                                          420
C                                                                      421
C - - END OF M.C. PROFILE ROUTINE - - - - - - - - - - - - - - - - -   422
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -   423
C                                                                      424
      CINC=0.0                                                         425
      CBARP=0.0                                                        426
      DO 795 I=1,N                                                     427
      CINC=CINC+(C(I)-CA(I))/N                                         428
  795 CBARP=CBARP+C(I)/N                                               429
      SORATE=CINC*(SG*A/100.)/DELT)                                    430
C - - THIS SORATE(IN G/SQ CM,TIME) IS FOR NPL LOOPS                   431
      WTCHNG=WTCHNG+SORATE*DELT                                        432
C - - THIS GIVES WEIGHT CHANGE(IN G/SQ CM) SINCE THE LAST DATA WRITE  433
C                                                                      434
      TIMET=TIMET+DELT                                                 435
      DELT8S=DELT8S+DELT8                                              436
C                                                                      437
      IF (IWRT.EQ.1.AND.ABS(CBARP-CBARP2).LT.WRT) GO TO 835           438
      IF (IWRT.EQ.2.AND.(TIMET-TST).LT.WRT) GO TO 835                 439
C                                                                      440
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -   441
C - - START OF WRITE ROUTINE - - - - - - - - - - - - - - - - - - - -  442
      TST=TST+WRT                                                      443
  805 CONTINUE                                                         444
      K=K+1                                                            445
      AVRATE=WTCHNG*100./(SG*A*(TIMET-TIMEK))                          446
C - - THIS GIVES AVRATE IN PERCENT/TIME.                              447
      CBARAV=0.5*(CBARP2+CBARP)                                        448
      RW=1.-RF1                                                        449
      DELTEF=100.*(TIMET-TIMEK)/DELT8S                                 450
      CBARP2=CBARP                                                     451
      TIMEK=TIMET                                                      452
C                                                                      453
      DO 815 I=1,10                                                    454
      LC=NCLM(I)                                                       455
  815 CWRITE(I)=C(LC)                                                  456
C                                                                      457
      WRITE (3,825) CBARP,TIMET,CBARAV,AVRATE,TW,RW,K,DELTEF,(CWRITE(I), 458
     1I=1,10)                                                          459
  825 FORMAT (1H ,1X,F6.2,1X,E10.4,1X,F7.3,1X,E10.4,1X,F6.2,1X,F5.3,1X,I 460
     13,1X,F7.3,10(1X,F6.2))                                          461
C                                                                      462
      WTCHNG=0.                                                        463
      DELT8S=0.0                                                       464
C - - END OF WRITE ROUTINE - - - - - - - - - - - - - - - - - - - - -  465
C - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -   466
  835 CONTINUE                                                         467
C                                                                      468
      IF (ABS(CBARP-EMC).LT.FINIS) GO TO 855                          469
  845 CONTINUE                                                         470
  855 CONTINUE                                                         471
      WRITE (3,865)                                                    472
      WRITE (3,875) J,NPL                                              473
  865 FORMAT (T1,'0',T126,'J',T131,'NPL')                            474
  875 FORMAT (T1,' ',T120,I7,T129,I5)                                 475
      GO TO 5                                                          476
  885 CONTINUE                                                         477
      CALL EXIT                                                        478
      END                                                             479
```