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DIFFUSE:

**A FORTRAN Program for Design Computation of
Tritium Transport through Thermonuclear
Reactor Components by Combined Ordinary and
Thermal Diffusion When the Principal Resistance to
Diffusion is the Bulk Metal**

John H. Pendergrass

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DIFFUSE:

**A FORTRAN PROGRAM FOR DESIGN COMPUTATION
OF TRITIUM TRANSPORT THROUGH THERMONUCLEAR
REACTOR COMPONENTS BY COMBINED ORDINARY AND
THERMAL DIFFUSION WHEN THE PRINCIPAL RESISTANCE
TO DIFFUSION IS THE BULK METAL**

by

John H. Pendergrass

ABSTRACT

Based on the theory developed in an earlier report, a FORTRAN computer program, DIFFUSE, was written. It computes, for design purposes, rates of transport of hydrogen isotopes by temperature-dependent, quasi-unidirectional, and quasi-static combined ordinary and thermal diffusion through thin, hot thermonuclear reactor components that can be represented by composites of plane, cylindrical-shell, and spherical-shell elements when the dominant resistance to transfer is that of the bulk metal. The program is described, directions for its use are given, and a listing of the program, together with sample problem results, is presented.

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ASSUMPTIONS, APPROXIMATIONS, AND THEORY

Detailed development of the theory is presented in the report LA-6542-MS¹ and will not be repeated here. The geometries that

can be accommodated are illustrated in Fig. 1. The basic approximations and assumptions involved include:

1. The temperature dependence of the ordinary diffusivity is adequately represented by an Arrhenius-type expression.
2. The temperature dependence of the heat of transport is adequately approximated by a linear expression in temperature.
3. The temperature dependence of the thermal conductivity may be neglected.
4. The resistances to hydrogen transport other than that of the bulk barrier material may be neglected.
5. Sieverts' law adequately describes hydrogen isotope solubility in barrier materials.
6. The hydrogen transport is quasi-static and quasi-unidirectional.
7. Laser-fusion reactor components can be adequately approximated as composites of plane, cylindrical-shell, and spherical-shell elements.
8. Physicochemical properties are not functions of direction.
9. Fick's law of diffusion is valid.
10. Simultaneously diffusing hydrogen isotopes do not interfere with one another.
11. Hydrogen isotope concentrations and fluxes are small.

The theory may be summarized as follows for the most complex case. In terms of concentrations

$$J = D_o \frac{(T_1 - T_2)}{(X_2 - X_1)} F_3 (C_1 - C_2) ,$$

Fig. 1.

(a) Plane barrier, (b) cylindrical-shell barrier, and (c) spherical-shell barrier.

$$J_{\theta L} = D_0 \frac{(T_1 - T_2)}{\ln(r_2/r_1)} F_3(C_1 - C_2) ,$$

$$J_{\Omega} = D_0 \frac{(T_1 - T_2)r_1 r_2}{(r_2 - r_1)} F_3(C_1 - C_2) ,$$

and

$$J = \int_A J dA ,$$

$$J = \theta \int_0^L J_{\theta L} d\ell ,$$

$$J = \int_{\Omega} J_{\Omega} d\omega ,$$

respectively, for plane, cylindrical-shell, and spherical-shell elements, where

$$F_3 = \frac{\frac{e^{-\frac{\alpha}{R} \tau_1}}{\frac{\beta}{R}} C_1 - \frac{e^{-\frac{\alpha}{R} \tau_2}}{\frac{\beta}{R}} C_2}{\frac{\tau_1}{(C_1 - C_2)\mu(\tau_2)}},$$

$$\mu(\tau_2) = \sum_{n=0}^{\infty} \left(\frac{Q_D - \alpha}{R} \right)^n \frac{\left(\tau_2^{\frac{\beta}{R}-1} - \tau_1^{\frac{\beta}{R}-1} \right)}{n! \left(n - \frac{\beta}{R} - 1 \right)},$$

and

J = hydrogen isotope flux, $[ML^{-2}\theta^{-1}]$

$J_{\theta L}$ = hydrogen isotope flux, $[ML^{-1}\theta^{-1}]$

J_{Ω} = hydrogen isotope flux, $[M\theta^{-1}]$

θ = angle, dimensionless

Ω = solid angle, dimensionless

ω = solid angle, dimensionless

L = length, $[L]$

l = length variable, $[L]$

D_0 = preexponential factor in Arrhenius expression for diffusivity, $[L^2\theta^{-1}]$

Q_D = exponential factor in Arrhenius expression for diffusivity, $[L^2\theta^{-1}]$

T_1 = barrier face temperature, $[T]$

T_2 = barrier face temperature, $[T]$

x_1 = barrier face location, $[L]$

x_2 = barrier face location, $[L]$

r_1 = barrier inner radius, $[L]$

r_2 = barrier outer radius, $[L]$

- C_1 = barrier face hydrogen isotope concentrations, $[ML^{-3}]$
 C_2 = barrier face hydrogen isotope concentration, $[ML^{-3}]$
 J = hydrogen isotope permeation rate, $[M\theta^{-1}]$
 τ_1 = $1/\gamma_1$, $[T^{-1}]$
 τ_2 = $1/T_2$, $[T^{-1}]$
 α = constant term in linear expression for temperature dependence of heat of transport, $[L^2\theta^2]$
 β = temperature coefficient in linear expression for temperature dependence of heat of transport, $[L^2\theta^{-2}T^{-1}]$
 R = ideal gas constant, $[L^2\theta^{-2}T^{-1}]$.

The relationship between hydrogen isotope concentration in the barrier material and the hydrogen isotope fugacity (partial pressure) is given by Sieverts' law:

$$C = S_0 e^{Q_S/RT} p^{1/2} ,$$

where

- C = hydrogen isotope concentration, $[ML^{-3}]$
 S_0 = preexponential factor, $[M^{1/2}L^{-5/2}\theta]$
 Q_S = exponential factor, $[L^2\theta^{-2}]$
 p = partial pressure, $[ML^{-1}\theta^{-2}]$
 T = temperature, $[T]$
 R = ideal gas constant, $[L^2\theta^{-2}T^{-1}]$.

Note that the program DIFFUSE still computes meaningful results if $\beta=0$, corresponding to a constant heat of transport, or if $\alpha=0$ and $\beta=0$, corresponding to no thermal diffusion.

For these simpler cases the theory for the fluxes involves respective replacement of F_3 by

$$F_2 = - \frac{e^{-\frac{\alpha}{R} \tau_1} C_1 - e^{-\frac{\alpha}{R} \tau_2} C_2}{(C_1 - C_2) \left\{ \xi \left[\frac{(Q_D - \alpha)}{R} \tau_2 \right] + \frac{(Q_D - \alpha)}{R} \eta \left[\frac{(Q_D - \alpha)}{R} \tau_2 \right] \right\}}$$

and

$$F_1 = - \frac{1}{\xi \left(\frac{Q_D}{R} \tau_2 \right) + \frac{Q_D}{R} \eta \left(\frac{Q_D}{R} \tau_2 \right)},$$

where

$$\xi(\lambda\tau) = \frac{e^{\lambda\tau}}{\tau} - \frac{e^{\lambda\tau_1}}{\tau_1}, \quad \eta(\lambda\tau) = E_1(-\lambda\tau) - E_1(-\lambda\tau_1),$$

$$E_1(z) = \int_z^\infty \frac{e^{-u}}{u} du,$$

and

λ = dummy variable, $[T]$

μ = dimensionless dummy variable.

REFERENCES

1. John Pendergrass, "Temperature-Dependent Ordinary and Thermal Diffusion of Hydrogen Isotopes through Thermonuclear Reactor Components," Los Alamos Scientific Laboratory report LA-6542-MS (October 1976).


```

      PROGRAM DIFFUSE(INP,OUT)
1  FORMAT(1H1,/)
2  FORMAT(1X,13(1H*),/,1X,13(1H*),/,1X,13(1H*),/,1X,13(1H*),/,1X,
   113(1H*))
3  FORMAT(1X,13(1H*),/,1X,13(1H*),105X,13(1H*),/,1X,13(1H*),45X,15HP
   PROGRAM DIFFUSE,45X,13(1H*),/,1X,13(1H*),105X,13(1H*),/,1X,13(1H*),
   26X,92HCOMBINED ORDINARY AND THERMAL DIFFUSION OF HYDROGEN ISOTOPES
   3 THROUGH THIN, HOT THERMONUCLEAR,7X,13(1H*),/,1X,13(1H*),6X,91HREA
   4CTOR COMPONENTS WHICH CAN BE APPROXIMATED BY COMPOSITES OF PLANE,
   5CYLINDRICAL SHELL, AND,8X,13(1H*),/,1X,13(1H*),5X,95HSPHERICAL-SHE
   6LL ELEMENTS WITH ARRHENIUS-TYPE DEPENDENCE OF ORDINARY DIFFUSIVITY
   7 ON TEMPERATURE,5X,13(1H*),/,1X,13(1H*),6X,92HLINEAR DEPENDENCE O
   8F HEAT OF TRANSPORT ON TEMPERATURE, AND TEMPERATURE DEPENDENCE OF
   9THERMAL,7X,13(1H*),/,1X,13(1H*),9X,85HCONDUCTIVITY NEGLIGIBLE AND
   10AQUASI-UNIDIRECTIONAL, QUASI-STEADY HEAT AND MASS TRANSFER,11X,13(1
   11H*),/,1X,13(1H*),105X,13(1H*),/,1X,13(1H*))
4  FORMAT(1X,13(1H*),/,1X,13(1H*),104X,14(1H*),/,1X,13(1H*),6X,92HMY
   12ORGEN ISOTOPE CONCENTRATIONS MAY BE EXPRESSED IN TERMS OF DISSOLV
   13ED ATOMIC CONCENTRATIONS,6X,14(1H*),/,1X,13(1H*),4X,92HIN BARRIER
   14MATERIALS OR AS HYDROGEN MOLECULE PARTIAL PRESSURES IN OR OVER PHA
   15SES ADJACENT TO,6X,14(1H*),/,1X,13(1H*),7X,89HBARRIER WHEN THE PRI
   16NCIPAL RESISTANCE TO TRANSFER IS DUE TO THE BULK BARRIER MATERIAL
   17AND,8X,14(1H*),/,1X,13(1H*),17X,70HORDINARY OR COMBINED ORDINARY A
   18ND THERMAL DIFFUSION CAN BE ACCOMMODATED,17X,14(1H*),/,1X,13(1H*),1
   19804X,14(1H*),/,1X,13(1H*))
5  FORMAT(1X,13(1H*),/,1X,52(1H*),26X,53(1H*),/,1X,52(1H*),5X,16HJOH
   20N PENETRAGRASS,5X,53(1H*),/,1X,52(1H*),26X,53(1H*),/,1X,13(1H*))
6  FORMAT(1X,13(1H*),/,1X,44(1H*),42X,45(1H*),/,1X,44(1H*),17X,9HGR0
   21UP L-5,16X,45(1H*),/,1X,44(1H*),42X,45(1H*),/,1X,44(1H*),5X,32H10S
   22P ALAMOS SCIENTIFIC LABORATORY,5X,45(1H*),/,1X,44(1H*),42X,45(1H*),
   233/,1X,44(1H*),19X,4H1977,19X,45(1H*),/,1X,44(1H*),42X,45(1H*),/,1X,
   24413(1H*))
7  FORMAT(16T5)
8  FORMAT(10A8)
9  FORMAT(5E15,5)
12 FORMAT(20H1COMPONENT NUMBER = ,13,/)
11 FORMAT(1X,10A8,/,1X,10A8,/)
12 FORMAT(46H ELEMENT ELEMENT
13 FORMAT(54H NUMBER TYPE FIRST SECOND THIRD)
14 FORMAT(60H CM. CM. CM. OR CTERAD
   15IANS,/)
15 FORMAT(15,A8,3X,F12,5,2X,E12,5,2X,F12,5)
16 FORMAT(///,60H ELEMENT ELEMENT TEMPERATURES ELEMENT CONCEN
   17TRATIONS)
17 FORMAT(58H NUMBER FIRST SECOND FIRST SEC0
   18ND)
18 FORMAT(61H DEG.KELVIN DEG.KELVIN G-ATOMS/CC. G-ATOM
   19S/CC.,/)
19 FORMAT(15,5X,4(F12,5,1X))
20 FORMAT(///,60H ELEMENT ORDINARY MASS DIFFUSIVITY HEAT OF T
   21RANSFERT)

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21 FORMAT(65H NUMBER PREFIXPOENTIAL EXPONENTIAL CONSTANT TERM TE D 52
TEMPERATURE) D 53
22 FORMAT(65H FACTOR FACTOR CO D 54
EFFICIENT) D 55
23 FORMAT(66H SQ.CM./SEC. G-CAL./G-ATOM G-CAL./G-ATOM G-C D 56
1AL/G-ATOM=) D 57
24 FORMAT(64H DE D 58
1G.KELVIN./) D 59
25 FORMAT(15.4X,E12.5,3X,E12.5,2X,E12.5,3X,E12.5) D 60
26 FORMAT(///.65H ELEMENT ELEMENT PARTIAL PRESSURES SIFVERTS D 61
1LAW CONSTANTS) D 62
27 FORMAT(70H NUMBER FIRST SECOND PREEXPONENTIAL D 63
1 EXPONENTIAL) D 64
28 FORMAT(71H TORR TORR G-ATOM/CC.SQRT(TORR) D 65
1 G-CAL./G-ATOM./) D 66
29 FORMAT(15.3X,E12.5,3X,E12.5,4X,E12.5,7X,E12.5) D 67
30 FORMAT(///.28H ELEMENT RATE OF PERMEATION) D 68
31 FORMAT(28H NUMBER OF HYDROGEN ISOTOPE) D 69
32 FORMAT(26H THROUGH ELEMENT) D 70
33 FORMAT(25H G-ATOMS/SEC./) D 71
34 FORMAT(15.7X,E12.5) D 72
35 FORMAT(///.66H TOTAL RATE OF PERMEATION OF HYDROGEN ISOTOPE THROUG D 73
1H COMPONENT = ,E12.5,13H G-ATOMS/SEC.) D 74
DIMENSION CAPTION(20),DD(50),DD(50),QTRANS1(50),QTRANS2(50),CONC1( D 75
150),CONC2(50),TEMP1(50),TEMP2(50),DIMEN1(50),DIMEN2(50),DIMEN3(50) D 76
2,ATYPE(3),PRESS1(50),PRESS2(50),SQ(50),OS(50) D 77
DATA (ATYPE(1),I=1,3) /RH PL,8H CS,8H SS/ D 78
DOUBLE PRECISION TINV1,TINV2,F1,F2,IFACTN,NN,M,SUM,LF1,LTINV1,TINV D 79
121 D 80
INTEGER ELTYPE(50) D 81
R = 1.987 D 82
PRINT 1 D 83
PRINT 2 D 84
PRINT 3 D 85
PRINT 2 D 86
PRINT 4 D 87
PRINT 2 D 88
PRINT 5 D 89
PRINT 2 D 90
PRINT 6 D 91
PRINT 2 D 92
READ 7,NCOMPS D 93
DO 63 NCOMP = 1,NCOMPS D 94
READ 8,(CAPTION(NCAP),NCAPT=1,20) D 95
READ 7,NFLEMS,KCHOICE D 96
READ 7,(ELTYPE(NFLEM),NFLEM=1,NFLEMS) D 97
READ 9,((DD(NFLEM),DD(NFLEM),QTRANS1(NFLEM),QTRANS2(NFLEM),BLANK), D 98
1NFLEM=1,NFLEMS) D 99
READ 9,((CONC1(NFLEM),CONC2(NFLEM),TEMP1(NFLEM),TEMP2(NFLEM),BLANK D100
1),NFLEM=1,NFLEMS) D101
READ 9,((DIMEN1(NFLEM),DIMEN2(NFLEM),DIMEN3(NFLEM),BLANK,BLANK),NE D102
1FLEM=1,NFLEMS) D103
IF(KCHOICE.EQ.0) GO TO 50 D104
READ 9,((SQ(NFLEM),OS(NFLEM),PRESS1(NFLEM),PRESS2(NFLEM),BLANK),NE D105
1FLEM=1,NFLEMS) D106
DO 49 NFLEM = 1,NFLEMS D107
CONC1(NFLEM) = SQ(NFLEM)*EXP(= OS(NFLEM)/(R*TEMP1(NFLEM)))*SQRT(PR D108
ESS1(NFLEM)) D109
49 CONC2(NFLEM) = SQ(NFLEM)*EXP(= OS(NFLEM)/(R*TEMP2(NFLEM)))*SQRT(PR D110
ESS2(NFLEM)) D111
50 PRINT 10,NCOMP D112
PRINT 11,(CAPTION(NCAP),NCAPT=1,20) D113
PRINT 12 D114

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PRINT 13	D115
PRINT 14	D116
DO 51 NELEM = 1, NLEMS	D117
NTYPE = FTYPE(NELEM)	D118
51 PRINT 15, NELEM, ATYPE(NTYPE), DIMEN1(NELEM), DIMEN2(NELEM), DIMEN3(NELEM)	D119
1FM)	D120
PRINT 16	D121
PRINT 17	D122
PRINT 18	D123
DO 52 NELEM = 1, NLEMS	D124
52 PRINT 19, NELEM, TEMP1(NELEM), TEMP2(NELEM), CONC1(NELEM), CONC2(NELEM)	D125
PRINT 20	D126
PRINT 21	D127
PRINT 22	D128
PRINT 23	D129
PRINT 24	D130
DO 53 NELEM = 1, NLEMS	D131
53 PRINT 25, NELEM, DD(NELEM), QTRANS1(NELEM), QTRANS2(NELEM)	D132
IF(KCHOICE.FO.P) GO TO 55	D133
PRINT 26	D134
PRINT 27	D135
PRINT 28	D136
DO 54 NELEM = 1, NLEMS	D137
54 PRINT 29, NELEM, PRESS1(NELEM), PRESS2(NELEM), S0(NELEM), OS(NELEM)	D138
55 PRINT 30	D139
PRINT 31	D140
PRINT 32	D141
PRINT 33	D142
SUMFLOW = 0.0	D143
DO 62 NELEM = 1, NLEMS	D144
TINV1 = 1.0/TEMP1(NELEM)	D145
TINV2 = 1.0/TEMP2(NELEM)	D146
F1 = (DD(NELEM) - QTRANS1(NELEM))/R	D147
F2 = QTRANS2(NELEM)/R	D148
F3 = QTRANS1(NELEM)/R	D149
F4 = DD(NELEM)/R	D150
IF((ABS(F2).LT.1.0E-05).AND.(ABS(F3).LT.1.0E-05)) FF = - (CONC1(NELEM) - CONC2(NELEM))/(EXP(F4*TINV2)/TINV2 - EXP(F4*TINV1)/TINV1 +	D151
2F4*(F1 - F4*TINV2) - F1*(- F4*TINV1))	D152
IF((ABS(F2).LT.1.0E-05).AND.(ABS(F3).GE.1.0E-05)) FF = - (EXP(- F3	D153
1*TINV1)*CONC1(NELEM) - EXP(- F3*TINV2)*CONC2(NELEM))/(EXP(F1*TINV2	D154
2)/TINV2 - EXP(F1*TINV1)/TINV1 + F1*(F1 - F1*TINV2) - F1*(- F1*TINV1	D155
3))	D156
IF(ABS(F2).LT.1.0E-05) GO TO 57	D157
SUM = (TINV2**(- F2 - 1.0) - TINV1**(- F2 - 1.0))/(- F2 - 1.0)	D158
LEACTH = 0.0	D159
LTINV1 = 0.0G(TINV1)	D160
LF1 = 0.0G(F1)	D161
TINV21 = TINV2/TINV1	D162
DO 56 M = 1, 75	D163
M = M	D164
NN = M - F2 - 1.0	D165
LEACTH = LEACTH + 0.0G(M)	D166
56 SUM = SUM + (TINV21**NN + 1.0)*DEXP(M*LTINV1 + M*(F1 - LEACTH)/NN	D167
FF = (DEXP(- F3*TINV1)*CONC1(NELEM)/TINV1**F2 - DEXP(- F3*TINV2)*C	D168
2ONC2(NELEM)/TINV2**F2)/SUM	D169
57 NTYPE = FTYPE(NELEM)	D170
GO TO (58, 59, 60), NTYPE	D171
58 GEOM1 = 1.0/DIMEN1(NELEM)	D172
GEOM2 = DIMEN2(NELEM)*DIMEN3(NELEM)	D173
GO TO 61	D174
	D175

59	GEOM1 = 1.0/ALOG((DIMEN1(NFLEM) + DIMEN2(NELEM))/DIMEN2(NELEM))	D176
	GEOM2 = 6.283185307*DIMEN3(NFLEM)	D177
	GO TO 61	D178
60	GEOM1 = (DIMEN1(NFLEM) + DIMEN2(NFLEM))*DIMEN2(NFLEM)/DIMEN1(NFLEM)	D179
	1)	D180
	GEOM2 = DIMEN3(NFLEM)	D181
61	FLUX = GEOM1*FF*(TEMP1(NELEM) - TEMP2(NELEM))*D0(NELEM)	D182
	FLOW = FLUX*GEOM2	D183
	SUMFLOW = SUMFLOW + FLOW	D184
62	PRINT 34,NELEM,FLOW	D185
63	PRINT 35,SUMFLOW	D186
	END	D187
	FUNCTION F(X)	E 1
	IF(X.GF.1.0) E1 = (0.2677737343 + X*(0.6347608925 + X*(18.05901697	E 2
	130 + X*(0.5733287401 + X))) / (X*EXP(X)*13.9584969288 + X*(21.09065	E 3
	1330827 + X*(25.6329561487 + X*(9.573322345 + X)))	E 4
	IF((X.GF.=3.0).AND.(X.LT.1.0)) E1 = X*(0.9999999 + X*(-0.2500001 +	E 5
	1X*(0.04555682 + X*(-0.01041576 + X*(0.001664156 + X*(-0.0002335179	E 6
	2 + X*(0.00002928433 - X*(0.000001766345 + X*(0.0000007122452))))	E 7
	3))) = ALOG(ABS(X)) = 0.5772156649	E 8
	IF((X.GF.=0.0).AND.(X.LT.=3.0)) E1 = (1.0 - (248.6697 + X*(224.423	E 9
	14 + X*(32.43665 + X*(3.061037 + X*(0.05176245)))) / (180.7837 + X*(	E 10
	222.63818 + X*(38.93944 + X*(3.995161 + X)))) / (X*EXP(X))	E 11
	IF((X.GF.=174.0).AND.(X.LT.=9.0)) E1 = (1.0 - (674.567029 + X*(57.	E 12
	14118330 + X*(-6.05529232 - X))) / ((699.06552 + X*(841.654932 + X*(4	E 13
	29.3133893 + X*(-8.01957683 + X*(-0.099792040)))) / (X*EXP(X))	E 14
	IF(X.LT.=174.0) E1 = 0.0	E 15
	RETURN	E 16
	END	E 17

Variables List for Program DIFFUSE (Major Variables in Order of Appearance) and Corresponding Variables of Theory

R	ideal gas constant (R)
NCOMPS	number of reactor components to be treated
CAPTION(*)	caption for each component for identification
NELEM	element number
NELEMS	number of plane, cylindrical-shell, and spherical-shell elements of which reactor component is composed

KCHOICE	specifies whether or not hydrogen isotope concentrations are to be specified directly or computed from fugacities (partial pressures) using Sieverts' Law
ELTYPE(•)	element type (1 for plane, 2 for cylindrical-shell, and 3 for spherical-shell elements)
$D_0(•)$	ordinary mass diffusivity preexponential factor for hydrogen isotope and element material under consideration (D_0)
$Q_D(•)$	ordinary mass diffusivity exponential factor for hydrogen isotope and element material under consideration (Q_D)
QTRANS1(•)	constant term in linear expression for heat of transport for hydrogen isotope and element material under consideration (α)
QTRANS2(•)	temperature coefficient in linear expression for heat of transport for hydrogen isotope and element material under consideration (β)
BLANK	dummy variable which merely occupies a position so that one input format can be used for several types of data subsets
CONC1(•)	concentration of hydrogen isotope at face number 1 of element (C_1)
CONC2(•)	concentration of hydrogen isotope at face number 2 of element (C_2)
TEMP1(•)	temperature at face number 1 of element (T_1)
TEMP2(•)	temperature at face number 2 of element (T_2)

DIMEN1(•) first dimension of element (thickness in all cases)
 $(x_2 - x_1, r_2 - r_1)$

DIMEN2(•) second dimension of element (inner radius in cases
of cylindrical and spherical shells, length of an
equivalent edge in case of plane element) (l, r_1)

DIMEN3(•) third dimension of element (length of an equivalent
edge in case of plane element, length of element in
case of cylindrical shell, solid angle in
steradians in case of spherical shell) (l, Ω)

$S\phi(\bullet)$ Sieverts' law preexponential factor for hydrogen
isotope and element material under consideration
 (S_0)

QS(•) Sieverts' law exponential factor for hydrogen
isotope and element material under consideration
 (Q_s)

PRESS1(•) hydrogen isotope fugacity (partial pressure) at
face number 1 of element (p_1)

PRESS2(•) hydrogen isotope fugacity (partial pressure) at
face number 2 of element (p_2)

ATYPE(•) element type (PL for plane element, CS for
cylindrical-shell element, SS for spherical-shell
element)

SUMFLOW total hydrogen isotope permeation rate through component

TINV1 inverse of TEMP1(•) (τ_1)

TINV2 inverse of TEMP2(•) (τ_2)

F1 $(Q(\bullet) - Q_{\text{TRANS1}}(\bullet))/R ((Q_0 - \alpha)/R)$

F2 $(Q_{\text{TRANS2}}(\bullet))/R (\beta/R)$

F3	QTRANS1(•)/R (α/R)
F4	QD(•)/R (Q_D/R)
FF	factor B, C, D
E1(•)	standard function ($E_1(•)$)
SUM	summation of series A
LFACN	$\ln(n!)$
LTINV1	$\ln(\text{TINV1}(•))$
LF1	$\ln(F1)$
TINV21	$\text{TINV2}/\text{TINV1}$ (τ_2/τ_1)
N	index
GEOM1	geometric factor ($1.0/\text{DIMEN1}(•)$ for element of type 1, $1.0/\ln((\text{DIMEN1}(•)+\text{DIMEN2}(•))/\text{DIMEN2}(•))$ for element of type 2, $(\text{DIMEN1}(•)+\text{DIMEN2}(•)) \times \text{DIMEN2}(•)/\text{DIMEN1}(•)$ for element of type 3) ($1/(X_2-X_1)$, $1/\ln(r_2/r_1)$, or $1r_2/(r_2-r_1)$)
GEOM2(•)	geometric factor ($\text{DIMEN2}(•) \times \text{DIMEN3}(•)$ for element of type 1, $2\pi \times \text{DIMEN3}(•)$ for element of type 2, $\text{DIMEN3}(•)$ for element of type 3) (A , $2\pi l$, Ω)
FLUX	flux of hydrogen isotope through element ($\text{FF} \times \text{GEOM1} \times (\text{TEMP1}(•)-\text{TEMP2}(•)) \times D\phi(•)$)
FLOW	rate of permeation of hydrogen isotope through element ($\text{FLUX} \times \text{GEOM2}$)

$$A \sum_{n=0}^{\infty} \frac{\left(\frac{Q_D - \alpha}{R}\right)^n \left(\tau_2^{n-\frac{\beta}{R}-1} - \tau_1^{n-\frac{\beta}{R}-1}\right)}{n! \left(n - \frac{\beta}{R} - 1\right)},$$

$$B \quad \frac{e^{-\frac{\alpha}{R} \tau_1} C_1 - e^{-\frac{\alpha}{R} \tau_2} C_2}{\frac{\beta}{R} \tau_1} \quad ,$$

$$\sum_{n=0}^{\infty} \frac{\left(\frac{Q_D - \alpha}{R} \right)^n \left(\tau_2^{n-\frac{\beta}{R}-1} - \tau_1^{n-\frac{\beta}{R}-1} \right)}{n! \left(n - \frac{\beta}{R} - 1 \right)}$$

$$C \quad - \frac{(C_1 - C_2)}{\xi \left(\frac{Q_D}{R} \tau_2 \right) + \frac{Q_D}{R} \eta \left(\frac{Q_D}{R} \tau_2 \right)} \quad ,$$

$$D \quad - \frac{e^{-\frac{\alpha}{R} \tau_1} C_1 - e^{-\frac{\alpha}{R} \tau_2} C_2}{(C_1 - C_2) \left\{ \xi \left[\frac{(Q_D - \alpha)}{R} \tau_2 \right] + \frac{(Q_D - \alpha)}{R} \eta \left[\frac{(Q_D - \alpha)}{R} \tau_2 \right] \right\}} \quad .$$

DATA INPUT INSTRUCTIONS

<u>Data</u>	<u>Card</u>	<u>Type</u>	<u>Data</u>	<u>Required</u>
	1		NCOMPS, the number of reactor components, according to FORMAT (16I5)	
	2		CAPTION(NCAPT),NCAPT=1,20, a descriptive caption for each reactor component, according to FORMAT (10A8)	
	3		NELEMS,KCHOICE, the number of elements in each component and whether or not Sieverts' law is	

to be included in the analysis, according to
 FORMAT (16I5) (KCHOICE=0 if Sieverts' law is
 not to be included, nonzero otherwise)

4 ELTYPE(NELEM),NELEM=1,NELEMS, element types
 for each component, according to FORMAT (16I5)
 (1, 2, or 3 depending on whether the element
 type is plane, cylindrical-shell, or spherical-
 shell)

5 (DØ(NELEM),QD(NELEM),QTRANS1(NELEM),
 QTRANS2(NELEM),BLANK),NELEM=1,NELEMS),
 preexponential factor in Arrhenius expression
 for ordinary diffusivity, exponential factor
 in Arrhenius expression for ordinary
 diffusivity, constant term in linear
 expression for heat of transport, temperature
 coefficient in linear expression for heat of
 transport, according to FORMAT (5E15.5)

6 (CONC1(NELEM),CONC2(NELEM),TEMP1(NELEM),
 TEMP2(NELEM),BLANK),NELEM=1,NELEMS), first and
 second hydrogen isotope concentrations, first
 and second barrier face temperatures,
 according to FORMAT (5E15.5)

7 (DIMEN1(NELEM),DIMEN2(NELEM),DIMEN3(NELEM),
 BLANK,BLANK),NELEM=1,NELEMS), first second,
 and third element dimensions according to
 FORMAT(5E15.5) (first is barrier thickness,
 second is inner radius for cylindrical shell-

and spherical-shell elements and equivalent transverse dimension for plane element, and third is equivalent transverse dimension for plane element, length for cylindrical-shell element, and solid angle for spherical-shell element)

8 (SO(NELEM),QS(NELEM),PRESS1(NELEM),
PRESS2(NELEM),BLANK),NELEM=1,NELEMS,
preexponential factor in Sieverts law
expression, exponential factor in Sieverts'
law expression, first element partial
pressure, and second element partial pressure,
according to FORMAT(5E15.5) (required only if
KCHOICE is nonzero)

If NCOMPS is greater than 1 repeat input for data and card types
2-8.

SAMPLE DATA INPUT

```

1      4
2 plane, cylindrical-shell, and spherical-shell elements
3 zero heat of transport, concentrations specified
4      3      0
5      1      2      3
6      1.000000e-02      2.000000e+04
7      1.000000e-02      2.000000e+04
8      1.000000e-02      2.000000e+04
9      1.000000e-06      1.000000e-07      1.000000e+03      9.000000e+02
10     1.000000e-06      1.000000e-07      1.000000e+03      9.000000e+02
11     1.000000e-06      1.000000e-07      1.000000e+03      9.000000e+02
12     1.000000e+00      2.000000e+00      3.000000e+00
13     1.000000e+00      2.000000e+00      3.000000e+00
14     1.000000e+00      2.000000e+00      3.000000e+00
15 plane, cylindrical-shell, and spherical shell-elements
16 constant heat of transport, concentrations specified

```

```

17      3      0
18      1      2      3
19      1.000000e-02      2.000000e+04      -1.000000e+04
20      1.000000e-02      2.000000e+04      -1.000000e+04
21      1.000000e-02      2.000000e+04      -1.000000e+04
22      1.000000e-06      1.000000e-07      1.000000e+03      9.000000e+02
23      1.000000e-06      1.000000e-07      1.000000e+03      9.000000e+02
24      1.000000e-06      1.000000e-07      1.000000e+03      9.000000e+02
25      1.000000e+00      2.000000e+00      3.000000e+00
26      1.000000e+00      2.000000e+00      3.000000e+00
27      1.000000e+00      2.000000e+00      3.000000e+00
28 plane, cylindrical-shell, and spherical shell-elements
29 variable heat of transport, concentrations specified
30      3      0
31      1      2      3
32      1.000000e-02      2.000000e+04      -2.100000e+04      1.100000e+01
33      1.000000e-02      2.000000e+04      -2.100000e+04      1.100000e+01
34      1.000000e-02      2.000000e+04      -2.100000e+04      1.100000e+01
35      1.000000e-06      1.000000e-07      1.000000e+03      9.000000e+02
36      1.000000e-06      1.000000e-07      1.000000e+03      9.000000e+02
37      1.000000e-06      1.000000e-07      1.000000e+03      9.000000e+02
38      1.000000e+00      2.000000e+00      3.000000e+00
39      1.000000e+00      2.000000e+00      3.000000e+00
40      1.000000e+00      2.000000e+00      3.000000e+00
41 plane element only
42 variable heat of transport, partial pressures specified
43      1      1
44      1
45      1.000000e-02      2.000000e+04      -2.100000e+04      1.100000e+01
46      1.000000e-06      1.000000e-07      1.000000e+03      9.000000e+02
47      1.000000e+00      2.000000e+00      3.000000e+00
48      3.16230e+02      2.05890e+04      1.000000e-08      1.000000e-09

```

OUTPUT FOR EXAMPLE PROBLEM

COVERED ORDINARY AND THERMAL DIFFUSION OF HYDROGEN ISOTOPES THROUGH THIN, HOT THERMONUCLEAR
REACTOR COMPONENTS WHICH CAN BE APPROXIMATED BY COMPOSITES OF PLANE, CYLINDRICAL-SHELL, AND
SPHERICAL-SHELL ELEMENTS WITH ARRHENIUS-TYPE DEPENDENCE OF ORDINARY DIFFUSIVITY ON TEMPERATURE,
LINEAR DEPENDENCE OF HEAT OF TRANSPORT ON TEMPERATURE, AND TEMPERATURE DEPENDENCE OF THERMAL
CONDUCTIVITY NEGLECTIBLE AND QUASI-UNIDIRECTIONAL, QUASI-STEADY HEAT AND MASS TRANSFER.

PROGRAM DIFFUSE

HYDROGEN ISOTOPES CONCENTRATIONS MAY BE EXPRESSED IN TERMS OF DISSOLVED ATOMIC CONCENTRATIONS
IN BARRIER MATERIALS OR AS HYDROGEN MOLECULE PARTIAL PRESSURES IN OR OVER PHASES ADJACENT TO
BARRIER WHEN THE PRINCIPAL RESISTANCE TO TRANSFER IS DUE TO THE BULK BARRIER MATERIAL AND
ORDINARY OR COMBINED ORDINARY AND THERMAL DIFFUSION CAN BE ACCOMMODATED

JOHN PENNFRASS

GROUP L-5

LOS ALAMOS SCIENTIFIC LABORATORY

1977

COMPONENT NUMBER = 1

PLANE, CYLINDRICAL-SHELL, AND SPHERICAL SHELL-ELEMENTS
ZERO HEAT OF TRANSPORT, CONCENTRATIONS SPECIFIED

ELEMENT NUMBER	ELEMENT TYPE	ELEMENT DIMENSIONS		
		FIRST CM.	SECOND CM.	THIRD CM. OR STERADIANS
1	PL	.10000E+01	.20000E+01	.30000E+01
2	CS	.10000E+01	.20000E+01	.30000E+01
3	SS	.10000E+01	.20000E+01	.30000E+01

ELEMENT NUMBER	ELEMENT TEMPERATURES		ELEMENT CONCENTRATIONS	
	FIRST DEG. KELVIN	SECOND DEG. KELVIN	FIRST G-ATOMS/CC.	SECOND G-ATOMS/CC.
1	.10000E+04	.90000E+03	.10000E-05	.10000E-06
2	.10000E+04	.90000E+03	.10000E-05	.10000E-06
3	.10000E+04	.90000E+03	.10000E-05	.10000E-06

ELEMENT NUMBER	ORDINARY MASS DIFFUSIVITY		HEAT OF TRANSPORT	
	PREFEXPOENTIAL FACTOR SQ. CM./SEC.	EXPONENTIAL FACTOR G-CAL./G-ATOM	CONSTANT TERM G-CAL./G-ATOM	TEMPERATURE COEFFICIENT G-CAL./G-ATOM- DEG. KELVIN
1	.10000E-01	.20000E+05	-0.	-0.
2	.10000E-01	.20000E+05	-0.	-0.
3	.10000E-01	.20000E+05	-0.	-0.

ELEMENT RATE OF PERMEATION
NUMBER OF HYDROGEN ISOTOPE
THROUGH ELEMENT
G-ATOMS/SEC.

1	.12711E-11
2	.98444E-11
3	.38132E-11

TOTAL RATE OF PERMEATION OF HYDROGEN ISOTOPE THROUGH COMPONENT = .14933E-10 G-ATOMS/SEC.

COMPONENT NUMBER = 2

PLANE, CYLINDRICAL-SHELL, AND SPHERICAL-SHELL ELEMENTS
CONSTANT HEAT OF TRANSPORT, CONCENTRATIONS SPECIFIED

ELEMENT NUMBER	ELEMENT TYPE	ELEMENT DIMENSIONS		
		FIRST CM.	SECOND CM.	THIRD CM. OR STERADIANS
1	PI	.10000E+01	.20000E+01	.30000E+01
2	CS	.10000E+01	.20000E+01	.30000E+01
3	SS	.1	.20000E+01	.30000E+01

ELEMENT NUMBER	ELEMENT TEMPERATURES		ELEMENT CONCENTRATIONS	
	FIRST NEG. KELVIN	SECOND NEG. KELVIN	FIRST G-ATOMS/CC.	SECOND G-ATOMS/CC.
1	.10000E+04	.90000E+03	.10000E+05	.10000E+06
2	.10000E+04	.90000E+03	.10000E+05	.10000E+06
3	.10000E+04	.90000E+03	.10000E+05	.10000E+06

ELEMENT NUMBER	ORDINARY MASS DIFFUSIVITY		HEAT OF TRANSPORT	
	DIFFERENTIAL FACTOR SQ. CM./SEC.	EXPONENTIAL FACTOR G-CAL./G-ATOM	CONSTANT TERM G-CAL./G-ATOM	TEMPERATURE COEFFICIENT G-CAL./G-ATOM NEG. KELVIN
1	.10000E+01	.20000E+05	.10000E+05	.0
2	.10000E+01	.20000E+05	.10000E+05	.0
3	.10000E+01	.20000E+05	.10000E+05	.0

ELEMENT RATE OF PERMEATION
NUMBER OF HYDROGEN ISOTOPE
THROUGH ELEMENT
G-ATOMS/SEC.

1	.83468E-12
2	.64672E-11
3	.25849E-11

TOTAL RATE OF PERMEATION OF HYDROGEN ISOTOPE THROUGH COMPONENT = .98059E-11 G-ATOMS/SEC.

COMPONENT NUMBER = 3

PLANE, CYLINDRICAL-SHELL, AND SPHERICAL-SHELL ELEMENTS
VARIABLE HEAT OF TRANSPORT, CONCENTRATIONS SPECIFIED

ELEMENT NUMBER	ELEMENT TYPE	ELEMENT DIMENSIONS		
		FIRST CM.	SECOND CM.	THIRD CM. OR STERADTANS
1	PL	.10000E+01	.20000E+01	.30000E+01
2	CS	.10000E+01	.20000E+01	.30000E+01
3	SS	.10000E+01	.20000E+01	.30000E+01

ELEMENT NUMBER	ELEMENT TEMPERATURES		ELEMENT CONCENTRATIONS	
	FIRST DEG. KELVIN	SECOND DEG. KELVIN	FIRST G-ATOMS/CC.	SECOND G-ATOMS/CC.
1	.10000E+04	.90000E+03	.10000E-05	.10000E-06
2	.10000E+04	.90000E+03	.10000E-05	.10000E-06
3	.10000E+04	.90000E+03	.10000E-05	.10000E-06

ELEMENT NUMBER	ORDINARY MASS DIFFUSIVITY		HEAT OF TRANSPORT	
	PREFEXPONENTIAL FACTOR SQ. CM./SEC.	EXPONENTIAL FACTOR G-CAL./G-ATOM	CONSTANT TERM G-CAL./G-ATOM	TEMPERATURE COEFFICIENT G-CAL./G-ATOM- DEG. KELVIN
1	.10000E-01	.20000E+05	-.21000E+05	.11000E+02
2	.10000E-01	.20000E+05	-.21000E+05	.11000E+02
3	.10000E-01	.20000E+05	-.21000E+05	.11000E+02

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ELEMENT RATE OF PERMEATION
NUMBER OF HYDROGEN ISOTOPE
THROUGH ELEMENT
G-ATOMS/SEC.

1	.81677E-12
2	.63284E-11
3	.24503E-11

TOTAL RATE OF PERMEATION OF HYDROGEN ISOTOPE THROUGH COMPONENT = .95955E-11 G-ATOMS/SEC.

COMPONENT NUMBER = 1

PLANE ELEMENT ONLY
VARIABLE HEAT OF TRANSPORT, PARTIAL PRESSURES SPECIFIED

ELEMENT NUMBER	ELEMENT TYPE	ELEMENT DIMENSIONS		
		FIRST CM.	SECOND CM.	THIRD CM. OR STERADIAN
1	D1	.12000E+01	.20000E+01	.30000E+01

ELEMENT NUMBER	ELEMENT TEMPERATURES		ELEMENT CONCENTRATIONS	
	FIRST DEG.KELVIN	SECOND DEG.KELVIN	FIRST G-ATOMS/CC.	SECOND G-ATOMS/CC.
1	.12000E+00	.90000E+03	.99970E-06	.99976E-07

ELEMENT NUMBER	ORDINARY MASS DIFFUSIVITY		HEAT OF TRANSPORT	
	PREEXPONENTIAL SQ.CM./SEC.	EXPONENTIAL FACTOR G-CAL./G-ATOM DEG.KELVIN	CONSTANT TERM G-CAL./G-ATOM DEG.KELVIN	TEMPERATURE COEFFICIENT G-CAL./G-ATOM- DEG.KELVIN
1	.12000E+01	.20000E+05	-.21000E+05	.11000E+02

ELEMENT NUMBER	ELEMENT PARTIAL PRESSURES		STEEVTS LAW CONSTANTS	
	FIRST TORR	SECOND TORR	PREEXPONENTIAL G-ATOM/CC.SQRT(TORR)	EXPONENTIAL G-CAL./G-ATOM
1	.10000E+07	.10000E+08	.31623E+03	.20500E+05

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ELEMENT RATE OF PERMEATION
NUMBER OF HYDROGEN ISOTOPE
THROUGH ELEMENT
G-ATOMS/SEC.

.81662E-12

TOTAL RATE OF PERMEATION OF HYDROGEN ISOTOPE THROUGH COMPONENT 3 .81662E-12 G-ATOMS/SEC.
COMPLETE