COMPUTER PROGRAMME FOR PHILIPS NUMERICAL SOLUTION OF EQUATIONS OF THE DIFFUSION TYPE WITH DIFFUSIVITY CONCENTRATION-DEPENDENT

A. F. NIELSEN

THERMAL INSULATION LABORATORY
TECHNICAL UNIVERSITY OF DENMARK

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A. F. Nielsen

Thermal Insulation Laboratory
Technical University of Denmark

This programme gives a solution to the equation:

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial \psi}{\partial x}\right)$$

where the diffusivity (D) is known in dependence of the potential (ψ). It could be used for thermal problems, where D is the thermal diffusivity, x is the place, ψ is the temperature and t is the time, and for water intake in materials, where D is the moisture diffusivity and ψ is the moisture content. Other problems could also be solved with the same equation. In the following we will use the water intake as an example.

The initial condition is a constant moisture content (ψ_o). The length in the positive x-direction is supposed infinite. At the time t=0 the material is brought in contact with water at x=0, and the input is maintained for all t>0 at a constant moisture content (ψ_s).

When $D(\psi)$ is known the problem is to find the moisture content for any x and t. This is done by using the Boltzmann transformation $\lambda = x \cdot t^{-\frac{1}{2}}$. The problem is solved by an iteration method, where $\lambda(\psi)$ is calculated from $D(\psi)$. When $\lambda(\psi)$ is found the moisture distribution is found from:

$$x = \lambda(\psi) \cdot t^{\frac{1}{2}} \;, \quad t = t_1, \; t_2, \; t_3$$

The description of this iteration method is omitted here, as it could be found in Philips, J.R. 1955: Numerical solution of equations of the diffusion type with diffusivity concentration-dependent. Trans. Faraday Soc., vol. 51, p 885-892, or Kirkham, D. and W.L. Powers: Advanced Soil Physics, p 287-319.

The computer programme has been written in FORTRAN IV, and has been run at the computing center NEUCC, the Technical University of Denmark. It is done on a IBM 370/165 with a CALCOMP plotter. The time used for running is app. 6 sec with plotter (CLASS=A). If the plotter part of the programme is omitted (the part between the two comment cards in the list of the programme) it will take app. 1 sec (CLASS=W). The class information and the time are not the same for other centers. It could also be necessary to rewrite the plotter part for use in other places.

The next pages give a list of the programme:

****************** NEUCC XMONITOR **************

```
ÅJOB    LIST
      DIMENSION T(100),D(100),DH(100),RH(100),AL(100),TI(10),TS(10),TU(1
     U),TOV(10),TOW(10),BL(100)
      IT=0
      READ(5,32) (TOV(I),I=1,10)
      READ(5,32) (TOW(I),I=1,10)
   32 FORMAT(10A4)
      READ(5,1) NR,FAK,THO,THN,DEL
    1 FORMAT(I5,4F10.5)
      READ(5,2)(T(I),D(I),I=1,NR)
    2 FORMAT(2F10.5)
      WRITE(6,3) NR,THO,THN
    3 FORMAT(1H0,'PHILIP SOLUTION FOR HORIZONTAL INFILTRATION'//1H0,'NUM
     1BER OF VALUES =',I5/1H0,'MAX VALUE MOISTURE CONTENT =',E12.6/1H0,'
     2MIN VALUE MOISTURE CONTENT =',E12.6//)
      WRITE(6,51) (TOV(I),I=1,10)
      WRITE(6,51) (TOW(I),I=1,10)
   51 FORMAT(1H0,10A4)
      FUR=ABS(T(NR)-THN)
      FOR=ABS(T(1)-THO)
      IF(FOR.GT.0.01) GO TO 100
      IF(FUR.GT.0.01) GO TO 100
      DO 4 I=1,NR
    4 D(I)=D(I)*FAK
      NQ=NR-1
      NQQ=NR-2
      TD=(THO-THN)/NQ
      DMID=0.0
      DO 5 I=1,NQ
    5 DH(I)=(D(I)+D(I+1))/2.0
      FAC=2.*TD/((THO-THN)**2)
      DO 6 I=1,NR
    6 DMID=DMID+D(I)*(T(I)-THN)
      DMID=DMID*FAC
      RH(1)=2.0*NQ*SQRT(DMID/3.14159)
      AL(1)=0.0
   11 AL(2)=2.0*DH(1)/RH(1)
      IT=IT+1
      DO 7 I=2,NQQ
      RH(I)=RH(I-1)-AL(I)
      L=I+1
    7 AL(L)=AL(I)+DH(I)*2.0/RH(I)
      RH(NQ)=RH(NQQ)-AL(NQ)
      YA=AL(NQ)/(2.0*SQRT(DH(NQ)))
      AB=2.*YA*EXP(-YA*YA)
      AC=SQRT(3.14159)*ERFC(YA)
      AY=AB/AC-2.0*YA*YA
      RHE=0.5*AL(NQ)+2.0*DH(NQ)*AY/AL(NQ)
      FOR=RH(NQ)-RHE
      FNU=ABS(FOR)
      IF(FNU.LT.DEL) GO TO 50
      RH(1)=RH(1)-FOR*0.5
      GO TO 11
   50 CONTINUE
      WRITE(6,12) IT
   12 FORMAT(1H0,'NUMBER OF ITERATIONS =',I5//1H0,4X,'MOISTURE CONTENT',
     19X,'DIFFUSIVITY',12X,'LAMBDA',14X,'I-VALUE'/)
      WRITE(6,10)(T(I),D(I),AL(I),RH(I),I=1,NQ)
      WRITE(6,10) T(NR),D(NR)
   10 FORMAT(1H ,3E20.5/1H ,60X,1E20.5)
```

```
******************   NEUCC XMONITOR   **************

      READ(5,20)(TI(I),I=1,10)
   20 FORMAT(10F8.3)
      DO 21 I=1,10
   21 TS(I)=SQRT(TI(I))
      WRITE(6,13) (TI(I),I=1,10)
   13 FORMAT(1H0,'MOISTURE',9X,'X-VALUES AT THE TIMES GIVEN IN NEXT LINE
     1'/1H0,10X,10F10.1)
      DO 22 I=2,NQ
      DO 23 J=1,10
   23 TU(J)=TS(J)*AL(I)
      WRITE(6,25) T(I),(TU(J),J=1,10)
   25 FORMAT(1H0,11F10.3)
   22 CONTINUE
      READ(5,30)TLX,TFX,TSX,TIX,TTX
   30 FORMAT(4X,F4.0,F6.3,F6.3,F4.0,F4.0)
      READ(5,30)TLY,TFY,TSY,TIY,TTY
      READ(5,30) DLX,DFX,DSX,DIX,DTX
      READ(5,31) DLY,NLOG
   31 FORMAT(4X,F4.0,I5)
      WRITE(6,36) DLY,NLOG
   36 FORMAT(1H0,'PLOT OF DIFFUSIVITY'/1H0,'    LENGTH(MM)',2X,'LOG SCALE
     1'/3H0 Y,5X,F6.0,5X,'10**(',I3,')  MIN VALUE'/)
      WRITE(6,34) DLX,DFX,DSX,DIX,DTX
      DMIN=10.**NLOG
      DMAX=DMIN*1000.
      WRITE(6,35)
   35 FORMAT(1H0,'PLOT OF MOISTURE CONTENT VERSUS PLACE'/)
      WRITE(6,34)   TLX,TFX,TSX,TIX,TTX
   34 FORMAT(//15H      LENGTH(MM),2X,8HFIRST(X),2X,7HLAST(X),2X,8HINTERV
     *AL,2X,8HSIZE(MM)/3H0 X,5X,F6.0,5X,F5.3,4X,F6.3,4X,F4.0,5X,F4.0)
      WRITE(6,33)   TLY,TFY,TSY,TIY,TTY
   33 FORMAT(15H      LENGTH(MM),2X,8HFIRST(M),2X,7HLAST(M),2X,8HINTERVAL
     *,2X,8HSIZE(MM)/3H0 Y,5X,F6.0,5X,F6.3,4X,F6.3,4X,F4.0,5X,F4.0)
      DO 50 I=1,NR
      DH(I)=D(I)
      IF(DH(I).GT.DMAX) DH(I)=DMAX
      IF(DH(I).LT.DMIN) DH(I)=DMIN
      DH(I)=DH(I)/DMIN
   50 DH(I)=ALOG10(DH(I))
      XMAAL=DLX/(DSX-DFX)
      YMAAL=DLY/3.
      DLY2=DLY*2.0/3.0
      DLY1=DLY/3.0
C
      CALL PARALF(10.,70.)
      CALL DREJ90(3)
      CALL FACTOR(0.1)
      CALL PLOT(0.,0.,2)
      CALL PLOT(0.,DLY,1)
      CALL PLOT(DLX,DLY,1)
      CALL PLOT(DLX,0.,1)
      CALL PLOT(0.,DLY1,2)
      CALL PLOT(DLX,DLY1,1)
      CALL PLOT(0.,DLY2,2)
      CALL PLOT(DLX,DLY2,1)
      DXN=DFX+(DSX-DFX)/DIX
      DF=(DXN-DFX)*DIX/DLX
      CALL AXE(0.,0.,DLX,0.,DFX,DXN,DF,DTX,1,0,2,-1.,1.)
      AA=DLY+30.
      AB=DLY+20.
```

```
******************  N=UCC XMONITOR  *************

      AC=DLY+10.
      CALL SYMBOL(0.,AA,6.,TOV,0.,40)
      CALL SYMBOL(0.,AB,5.,TOW,0.,40)
      AD=FLOAT(NLOG)
      CALL SYMBOL(0.,AC,5.,21HLOWER LOG. VALUE 10**,0.,21)
      CALL NUMBER(110.,AC,5.,AD,0.,-1)
      CALL KURVE(T,DH,NR,1,XMAAL,YMAAL,0.,0.,-1,0,1.0)
      CALL PARALF(200.,0.)
      DO 41 J=1,10
      DO 40 I=2,NQ
   40 DH(I)=TS(J)*AL(I)
      DH(1)=0.0
      JJ=0
      DO 42 K=1,NG
      JJ=JJ+1
      IF(DH(K).GT.TSX.OR.DH(K).LT.TFX) JJ=JJ-1
      IF(DH(K).GT.TSX.OR.DH(K).LT.TFX) GO TO 42
      BL(JJ)=DH(K)
      RH(JJ)=T(K)
      JN=JJ
   42 CONTINUE
      IF(JN.LE.2) GO TO 41
      XMAAL=TLX/(TSX-TFX)
      YMAAL=TLY/(TSY-TFY)
      LIT=-1
      CALL KURVE(BL,RH,JN,1,XMAAL,YMAAL,TFX,TFY,LIT,I,1.0)
   41 CONTINUE
      TXN=TFX+(TSX-TFX)/TIX
      XF=(TXN-TFX)*TIX/TLX
      CALL AXE(0.,0.,TLX,0.,TFX,TXN,XF,TTX,1,0,2,-1.,1.)
      TYN=TFY+(TSY-TFY)/TIY
      YF=(TYN-TFY)*TIY/TLY
      CALL AXE(0.,0.,TLY,90.,TFY,TYN,YF,TTY,1,1,2,1.,1.)
      CALL PLTEND
C
      GO TO 150
  100 CONTINUE
      WRITE(6,101)(T(I),I=1,NR)
  101 FORMAT(1H0,6E20.5)
      WRITE(6,102)
  102 FORMAT(1H0,'WRONG INPUT DATA =')
  150 CONTINUE
      STOP
      END
```

Input data cards for the programme:

1. card	col 1-40	(10A4)	text first line of heading.
2. card	col 1-40	(10A4)	text second line of heading.
3. card	col 1-5	(I5)	number of diffusivity values.
	col 6-15	(F10.5)	multiplication factor of diffusivity.
	col 16-25	(F10.5)	saturated moisture content.
	col 26-35	(F10.5)	initial moisture content.
	col 36-45	(F10.5)	maximum error in the iteration (for the I-value).
4. card	col 1-10	(F10.5)	moisture content.
	col 11-20	(F10.5)	diffusivity $[L^2/T]$

5. to R. card like 4. card.
The total number of cards, moisture content versus diffusivity, should be as defined in card 3, col 1-5. The card should be placed in the order of decreasing value of moisture content. The difference in moisture content between two succeeding cards should be the same.

R+1 card The times when the moisture distribution is to be calculated. The time in min, sec and hours in which the diffusivity is given. Ten time values [T].

col 1-8	(F8.3)	first time.
col 9-16	(F8.3)	second time.

and so on, totally 10F8.3.

R+2 card x-axis for the moisture distribution plot.

col 5-8	(F4.0)	length of axis in mm.
col 9-14	(F6.3)	first value (length [L]).
col 15-20	(F6.3)	last value (length [L]).
col 21-24	(F4.0)	number of intervals.
col 25-28	(F4.0)	size of numbers in mm.

R+3 card y-axis for the moisture distribution plot.

col 5-8	(F4.0)	length of axis in mm.
col 9-14	(F6.3)	first value (moisture content).
col 15-20	(F6.3)	last value (moisture content).
col 21-24	(F4.0)	number of intervals
col 25-28	(F4.0)	size of numbers in mm.

R+4 card   x-axis for the diffusivity plot.

- col 5-8 (F4.0) length of axis in mm.
- col 9-14 (F6.3) first value (moisture content).
- col 15-20 (F6.3) last value (moisture content).
- col 21-24 (F4.0) number of intervals.
- col 25-28 (F4.0) size of numbers in mm.

R+5 card   y-axis for the diffusivity plot, 3 decades logarithmic scale.

- col 5-8 (F4.0) length of axis in mm.
- col 9-13 (I5) exponent (a) for the lower logarithmic value.

The axis is defined from 10^a to 10^{a+3}.

```
WATER DIFFUSIVITY CM2/MIN
PHILIP(1955) EXAMPLE 1
   11     1.0        1.0        0.0        0.01
    1.0     16.
    0.9     16.
    0.8     16.
    0.7     16.
    0.6     16.
    0.5   8.5
    0.4    1.0
    0.3    1.0
    0.2    1.0
    0.1    1.0
    0.0    1.0
    2.0     4.0     9.0    16.0    25.0    36.0    49.0    64.0    81.0    100.
XAX=250.    0.    25.    5.  4.
YAX=200.    0.     1.    5.  4.
YDAX100.    0.    01.    5.  4.
YDAX200.
```

<u>The printer output</u> is seen on next page and consists of:

The input data.
The number of iterations used to solve the equation is found.
For the moisture contents are found the λ-values and the I-values.
For the given times is for each moisture content found the x-value (place).
At last is given the values for the plotting.

<u>The plotter output</u> is shown in some of the examples.

PHILIP SOLUTION FOR HORIZONTAL INFILTRATION

NUMBER OF VALUES = 11

MAX VALUE MOISTURE CONTENT =0.100000E 01

MIN VALUE MOISTURE CONTENT =0.0

WATER DIFFUSIVITY CM2/MIN

PHILIP(1955) EXAMPLE 1

NUMBER OF ITERATIONS = 5

MOISTURE CONTENT	DIFFUSIVITY	LAMBDA	I-VALUE
0.10000E 01	0.16000E 02	0.0	0.37179E 02
0.90000E 00	0.16000E 02	0.86069E 00	0.36319E 02
0.80000E 00	0.16000E 02	0.17418E 01	0.34577E 02
0.70000E 00	0.16000E 02	0.26672E 01	0.31910E 02
0.60000E 00	0.16000E 02	0.36701E 01	0.28240E 02
0.50000E 00	0.85000E 01	0.48032E 01	0.23436E 02
0.40000E 00	0.10000E 01	0.48886E 01	0.18548E 02
0.30000E 00	0.10000E 01	0.49964E 01	0.13551E 02
0.20000E 00	0.10000E 01	0.51440E 01	0.84074E 01
0.10000E 00	0.10000E 01	0.53819E 01	0.30255E 01
0.0	0.10000E 01		

MOISTURE X-VALUES AT THE TIMES GIVEN IN NEXT LINE

MOISTURE	2.0	4.0	9.0	16.0	25.0	36.0	49.0	64.0	81.0	100.0
0.900	1.217	1.721	2.582	3.443	4.303	5.164	6.025	6.886	7.746	8.607
0.800	2.463	3.484	5.225	6.967	8.709	10.451	12.192	13.934	15.676	17.418
0.700	3.772	5.334	8.002	10.669	13.336	16.003	18.671	21.338	24.005	26.672
0.600	5.190	7.340	11.010	14.680	18.350	22.020	25.691	29.361	33.031	36.701
0.500	6.793	9.606	14.410	19.213	24.016	28.819	33.623	38.426	43.229	48.032
0.400	6.913	9.777	14.666	19.554	24.443	29.331	34.220	39.109	43.997	48.886
0.300	7.066	9.993	14.989	19.986	24.982	29.978	34.975	39.971	44.968	49.964
0.200	7.275	10.288	15.432	20.576	25.720	30.864	36.008	41.152	46.296	51.440
0.100	7.611	10.764	16.146	21.527	26.909	32.291	37.673	43.055	48.437	53.819

PLOT OF DIFFUSIVITY

	LENGTH(MM)	LOG SCALE	
Y	200.	10**(0)	MIN VALUE

	LENGTH(MM)	FIRST(X)	LAST(X)	INTERVAL	SIZE(MM)
X	100.	0.0	1.000	5.	4.

PLOT OF MOISTURE CONTENT VERSUS PLACE

	LENGTH(MM)	FIRST(X)	LAST(X)	INTERVAL	SIZE(MM)
X	250.	0.0	25.000	5.	4.
	LENGTH(MM)	FIRST(M)	LAST(M)	INTERVAL	SIZE(MM)
Y	200.	0.0	1.000	5.	4.

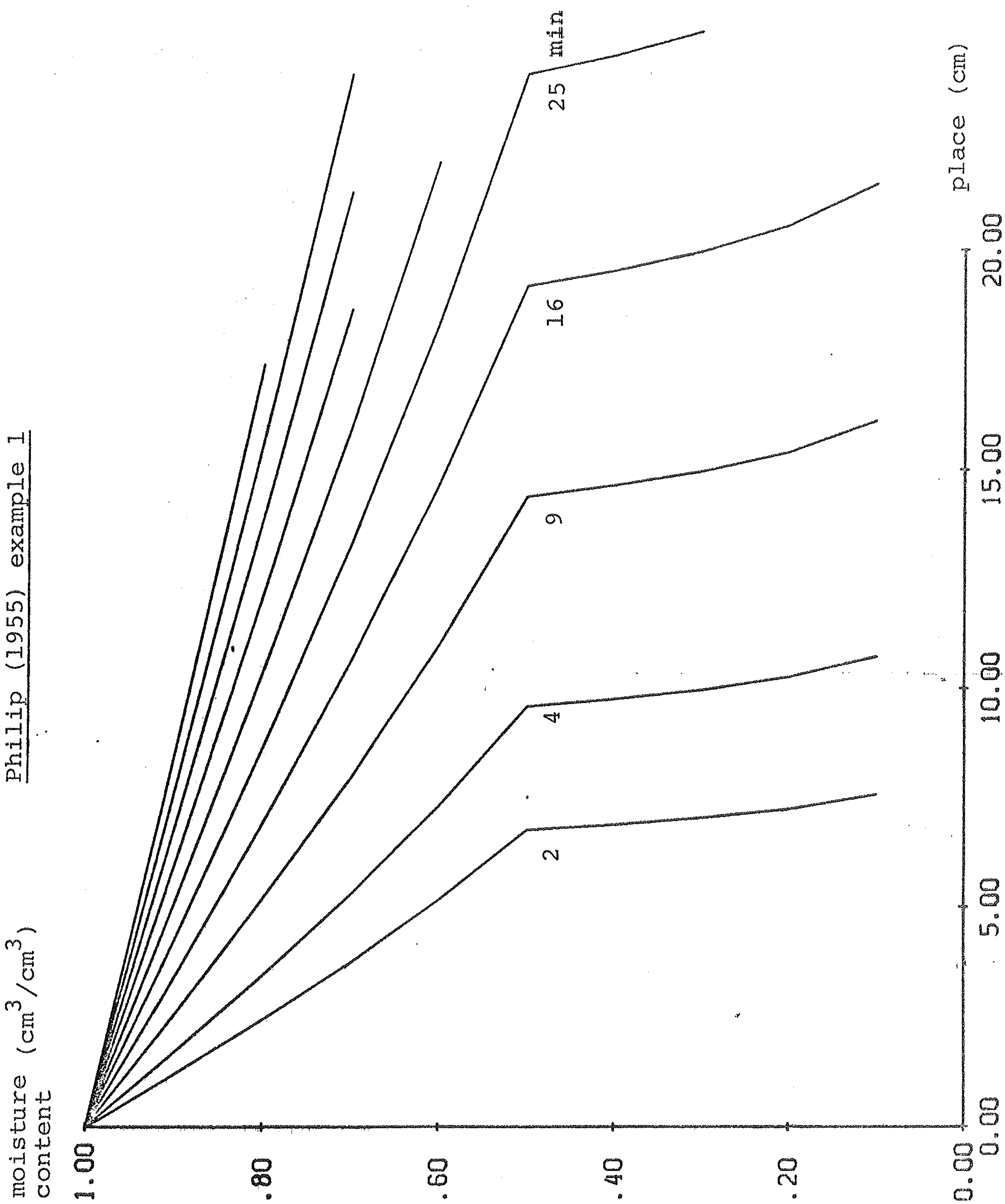
```
*PLOT* I;ROUTINE=PLTEND;MESSAGE=PLOTTING TERMINATED;
       VALUE=ESTIMATED PLOTTIME:=       9 MINS.  .
             ESTIMATED NOPLOTTIME:=     ? MINS.  .
             DIMENSION OF DRAWING:=    42 * 70 CM;
```

Examples

The first example is the same as calculated by Philip (1955), where the initial moisture content (ψ_o) is zero, and the saturated moisture content (ψ_s) is one. The diffusivity is 1 cm^2/min for $0 < \psi < 0.5$, and 16 cm^2/min for $0.5 < \psi < 1.0$. The computer programme gives the same results as can be seen by comparing the lambda values:

moisture content	λ-value, Philip	λ-value, programme
0.9	0.8607	0.8607
0.8	1.7418	1.7418
0.7	2.6674	2.6674
0.6	3.6705	3.6701
0.5	4.8042	4.8032
0.4	4.8896	4.8886
0.3	4.9977	4.9964
0.2	5.1462	5.1440
0.1	5.3884	5.3819

The difference is probably caused by a limited accuracy in the Philip calculation as quoted in Kirkham, p. 314. The resulting moisture distributions are given on next page. It should be pointed out that in this particular example the diffusivity plot is omitted. The printer output is found after the description of the output.


Philip (1955) example 1
moisture content (cm3/cm3)
1.00
.80
.60
.40
.20
0.00
0.00
5.00
10.00
15.00
20.00
place (cm)
2
4
9
16
25 min

Calculations of free-water intake on cellular concrete

The 3 next examples are an illustration of the use of the computer programme to get moisture distributions for different diffusivity curves.

The first example shows the calculation for a straight line connexion in a logarithmic scale. The diffusivity values are in the correct magnitude. The moisture diffusivity is found for the time t=2h, 4h, 9h, 16h, 25h, 36h, 49h, 64h, 81h and 100h.

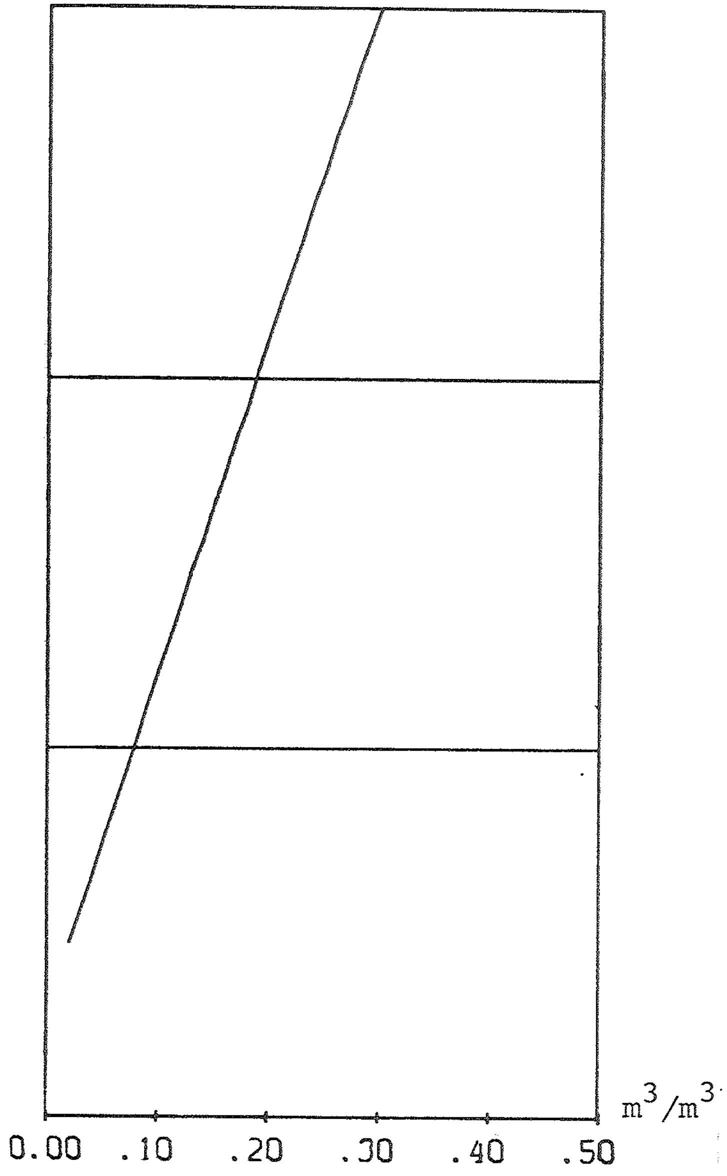
The second example shows calculations with diffusivity found in van der Kooi: Moisture Transfer in Cellular Concrete Roofs, Delft 1971. The same example as he uses in his computer programme. The moisture "front" is seen to be more vertical than in the first example. The rate of water intake is much lower.

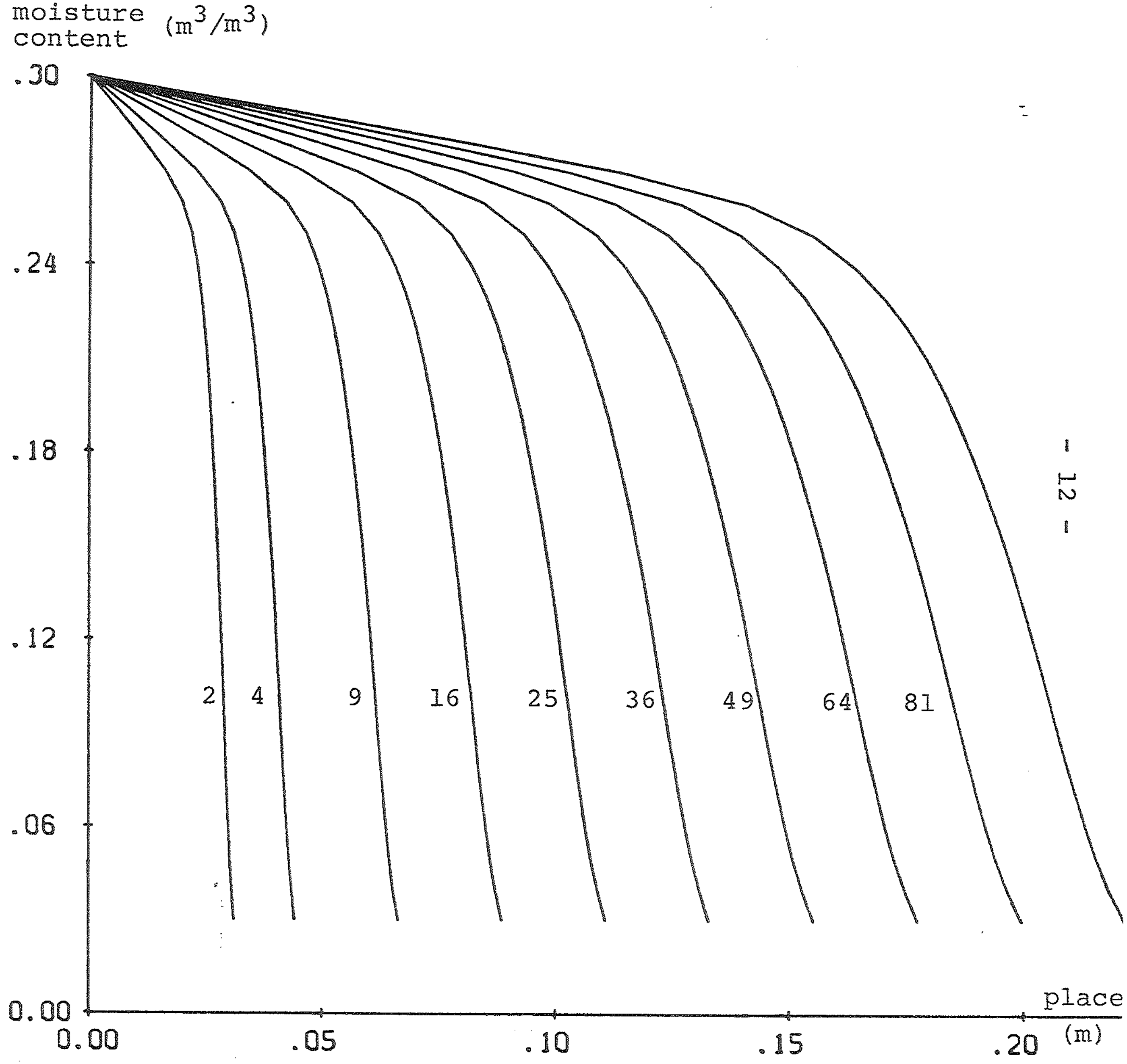
The third example shows calculations of diffusivity found by Bo Søgaard Nielsen in his unpublished diploma work at the Thermal Insulation Laboratory 1975. The diffusivity curve has been found from free-water intake experiments. The calculated moisture content from this curve shows a good correlation with experimental results, see last page. This is a little surprising, as the length of the specimen is 15 cm, and the theory is assuming infinite length.

WATER DIFFUSIVITY M2/H

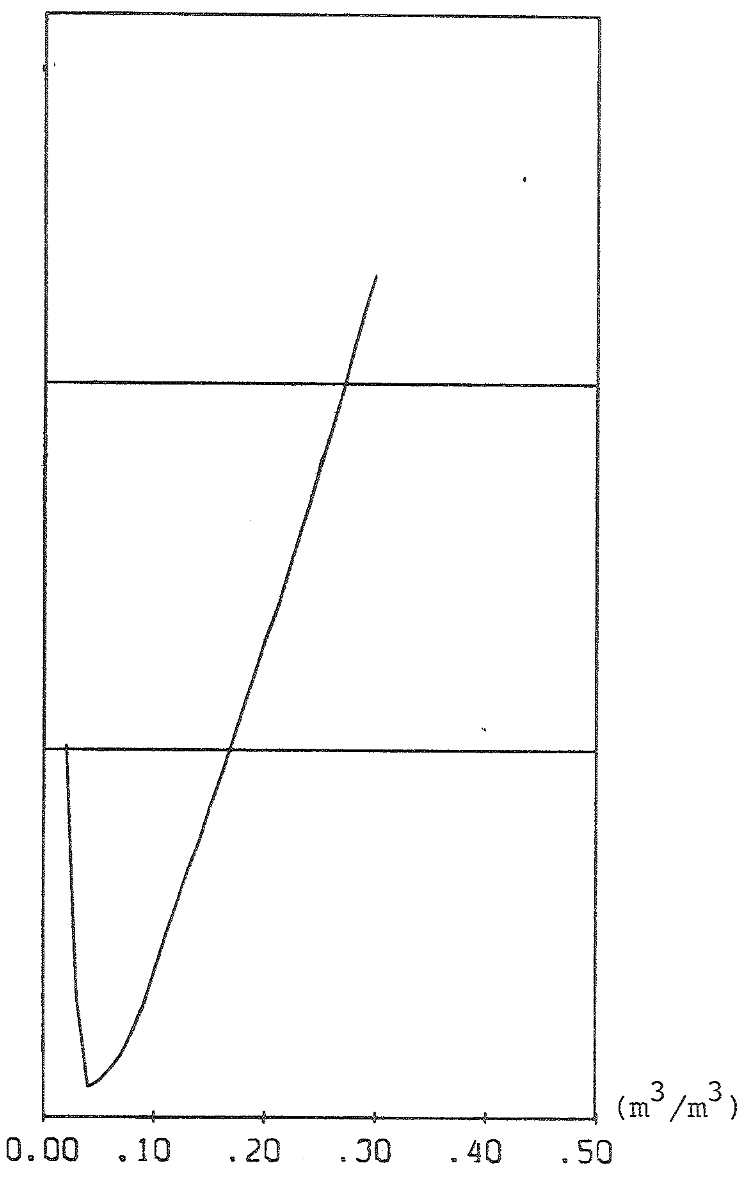
EXAMPLE 2

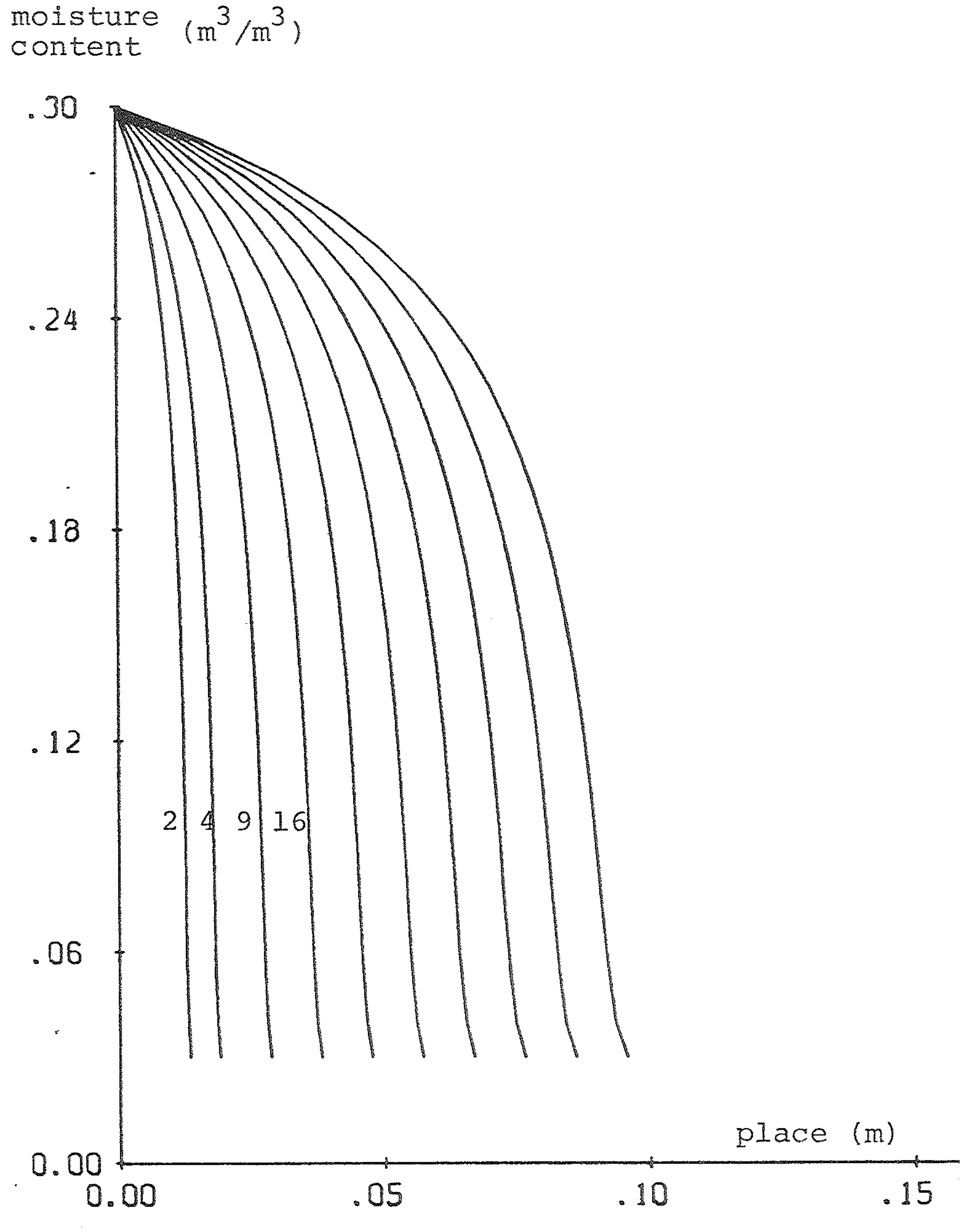
LOWER LOG. VALUE 10** -6



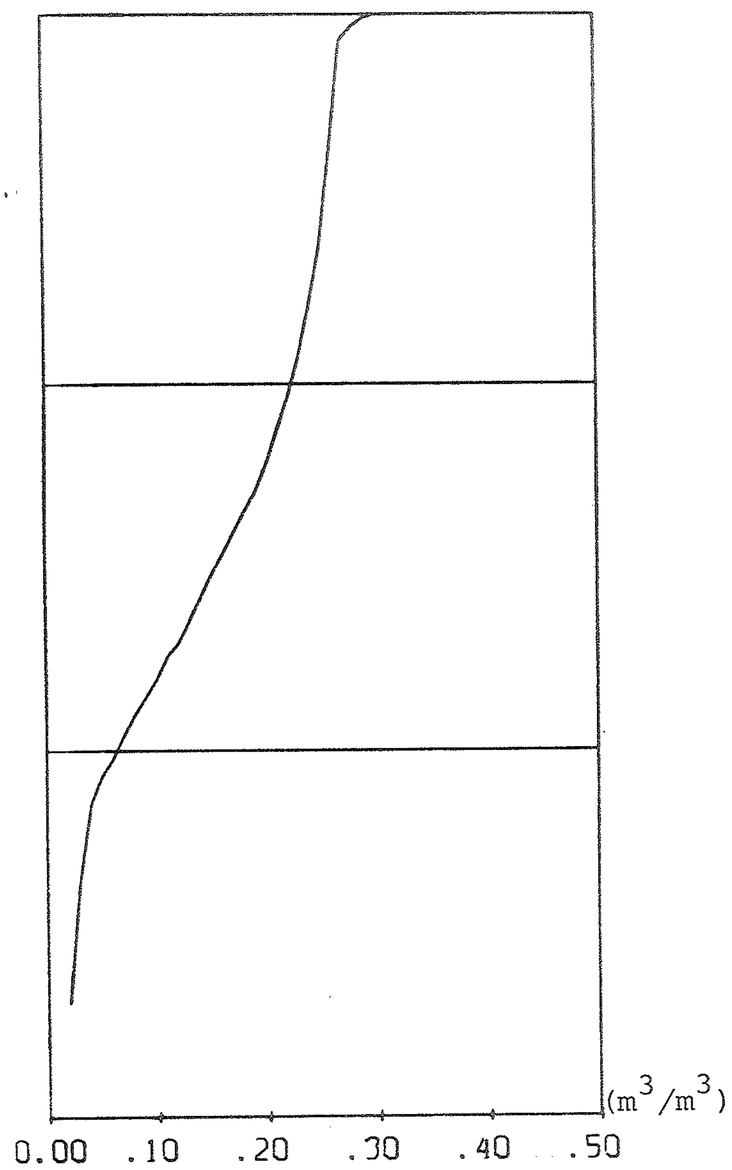


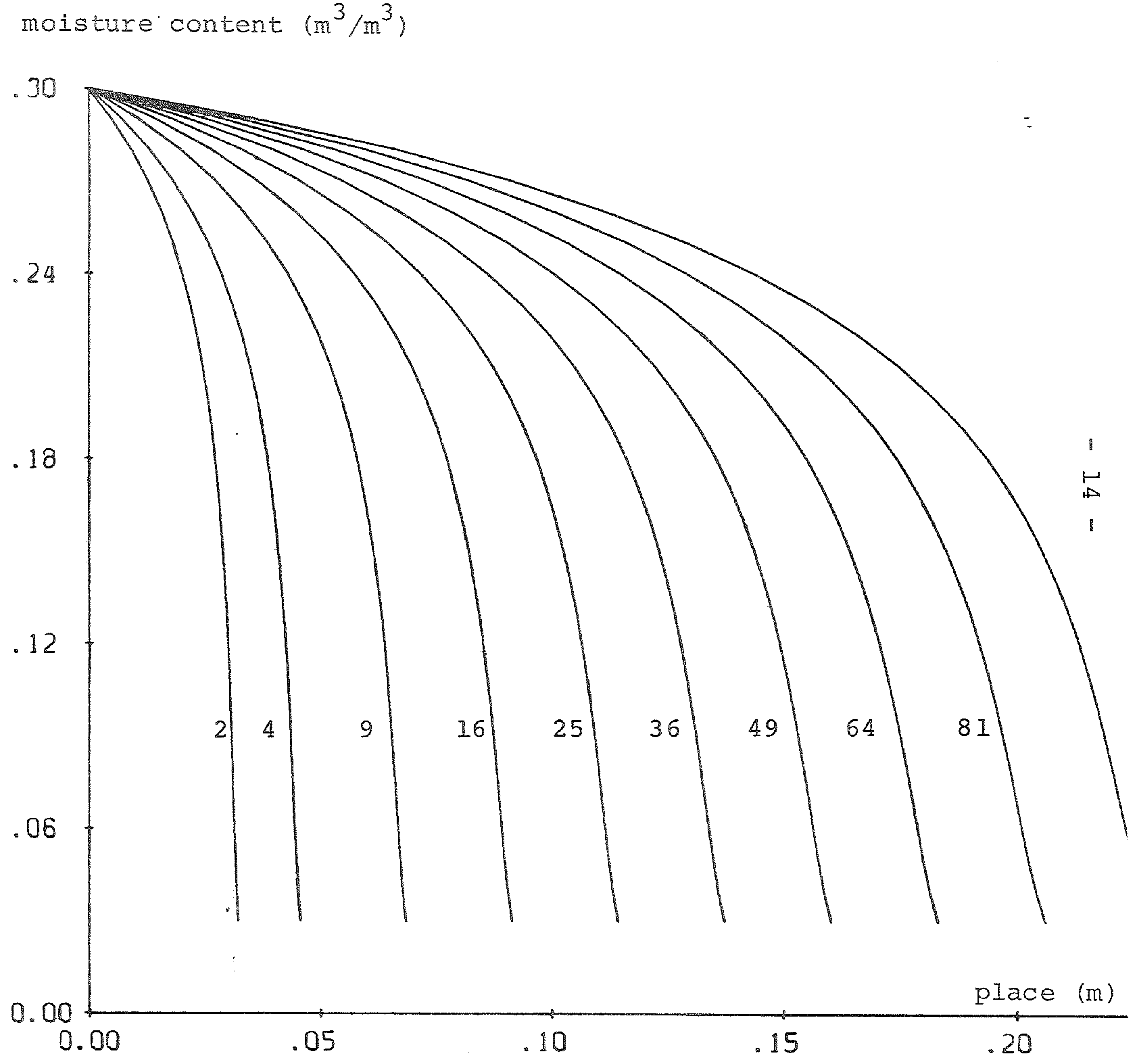
WATER DIFFUSIVITY M2/H
VAN DER KOOI COMPUTER VALUE
LOWER LOG. VALUE 10** -6

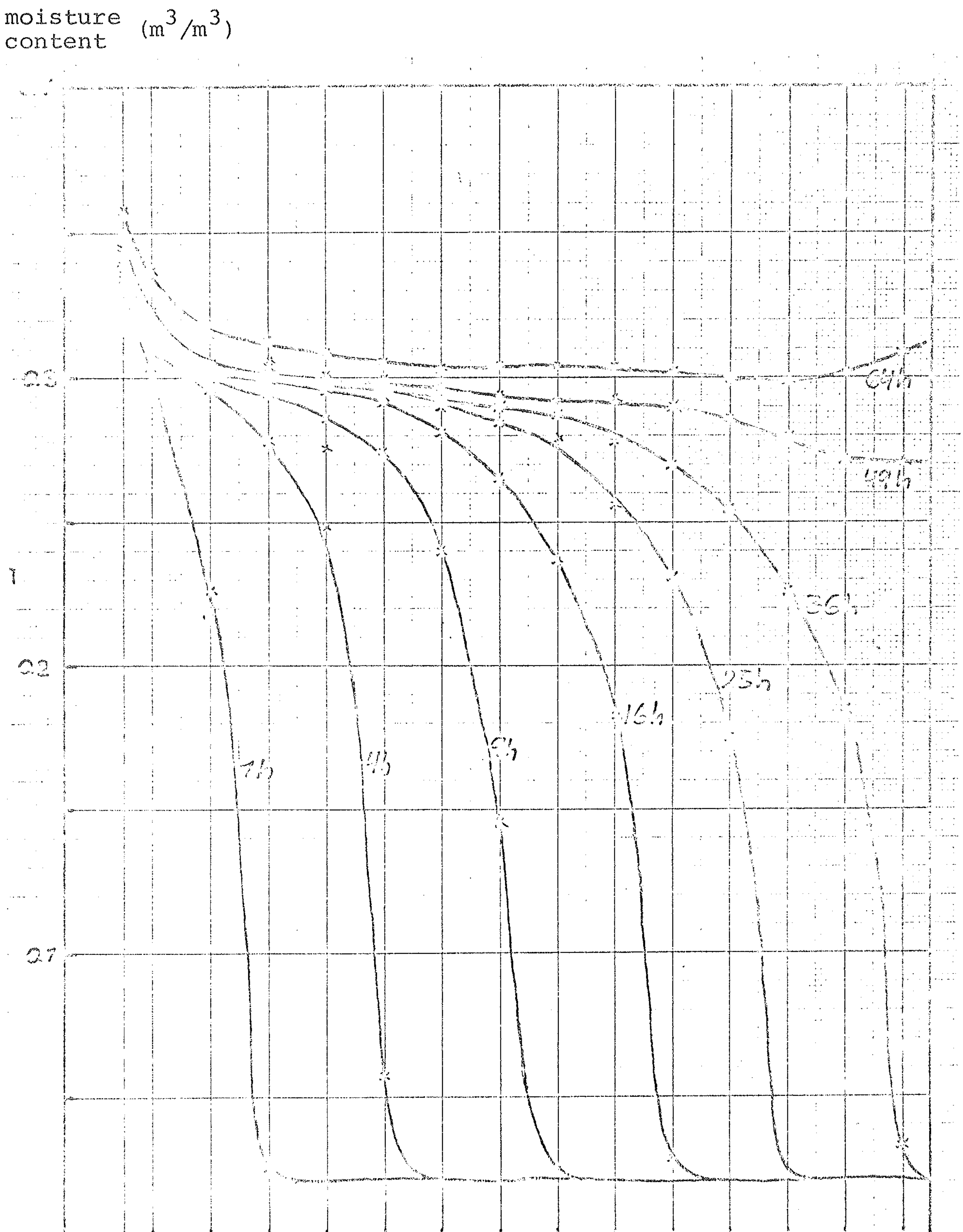




WATER DIFFUSIVITY M2/H
BO S@G$RD NIELSEN
LOWER LOG. VALUE 10** -6







Free-water intake on cellular concrete measured by gamma-ray-attenuation by Bo Søgaard Nielsen.