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DETERMINATION OF HYDRAULIC CONDUCTIVITY-CAPILLARY PRESSURE RELATIONSHIP
FROM SATURATION-CAPILLARY PRESSURE DATA FROM SOILS

A Description of a Computer Program for Numerically Evaluating the Burdine Integrals

By

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INTRODUCTION

Saturation (or moisture content) of soils has been studied and measured widely in the laboratory for many years. In more recent years such instruments as the neutron moisture meter or gamma probes have been developed for moisture content determinations. With these instruments field measurements as well as laboratory moisture contents can readily be obtained. A variety of tensiometers, osmotic devices, pressure transducers and psychrometric devices have also been developed for relatively rapid measurements of capillary pressure (a negative quantity), within partially saturated soil. With available instrumentation, therefore, saturation-pressure data can be obtained readily both in the field and the laboratory.

The hydraulic conductivity (or permeability) and capillary pressure relationship is vital in analyzing moisture movement through unsaturated soils. This latter relationship must be known to utilize a basic flow equation such as Darcy's Law. Unfortunately, measurements of hydraulic conductivity versus capillary pressure are difficult and time consuming to obtain in the laboratory and virtually impossible to obtain from field measurements.

Fortunately, theory proposed by Burdine (1953) is available for obtaining hydraulic conductivity capillary pressure
relationships from saturation-capillary pressure relationships. The approximations involved in this theory, which will be referred to hereafter as Burdine Theory or Burdine Integrals, as well as its uses, are discussed by Brooks and Corey (1964) and 1966) and Laliberte et al (1968). For further explanation of the Burdine Theory the reader should consult the references cited by these authors. In brief, the Burdine Theory gives reasonably accurate values of relative permeability from pressure saturation data. The result from the Burdine Theory is given by the following equation:

\[
k_r = \frac{k}{k_o} = S_e^2 \int_{S_r}^{1} \frac{ds}{S_r p^2} \int_{S_r}^{1} \frac{ds}{p^2}
\]

in which \( k_r \) is the relative intrinsic permeability with dimensions of length squared, \( k \) is the intrinsic permeability, \( k_o \) is the saturated intrinsic permeability, \( p \) is the capillary pressure (or pressure head), and \( S_e \) is the effective saturation defined by \( S_e = (S - S_r)/(1 - S_r) \), in which \( S_r \) is the residual saturation. Physically \( S_r \) is that value of saturation at which moisture movement ceases. Its value is generally determined, however, by achieving as good a fit as possible of data to a functional relationship of \( S_e \) versus capillary pressure. Actually \( k_r \) in
Eq. 1 may be interpreted as the relative hydraulic conductivity
\[ K_r = \left( \frac{\gamma g}{\mu} \right) k_r \]
with dimensions of velocity provided the density \( \gamma \) nor viscosity \( \mu \) of the fluid vary.

This paper describes a computer program (written in FORTRAN IV) which evaluates Equation 1 numerically using discrete data which define the saturation capillary pressure relationship for a given soil. Originally the program was developed as a SUBROUTINE in a program designed to solve problems of transient moisture movement from a circular infiltrometer during which solution values of relative hydraulic conductivity as well as its derivative with respect to the capillary pressure were required repeatedly (see Jeppson, 1970). Since a variety of needs exist for obtaining the permeability-pressure relationship from saturation-pressure data, the SUBROUTINE has been changed into a stand along program. The methodology used in evaluating the Burdine Integrals, as well as a description of the input to and output from the program are given herein.
METHOD OF SOLUTION

The computer program is designed to read data defining the saturation-pressure relationship. This data should define this relationship in a reasonably smooth fashion so that derivatives will be continuous within ranges over several consecutive data points. Should experimental error cause the data to exhibit an erratic behavior, it should be smoothed by some appropriate technique prior to supplying it as input to the program. From this data the program will evaluate the following quantities at each of a specified number of increments of pressure: (1) the saturation, \( S \), (2) the effective saturation, \( S_e' \), (3) the relative permeability, \( k_r' \), (4) \( (1/k_r')(\partial S/\partial p) \) and (5) \( (1/k_r')(\partial k_r/\partial p) \). The pressure increment between consecutively computed values is one-half as large over the first half of the total range as over the second half. These quantities are obtained by passing a second degree polynomial through each three consecutive data points supplied as input advancing one point at a time as necessary to evaluate Equation 1 over the entire range of the input data.

Lagrange's interpolation formula (see Kunz, 1957) has been used to define this second degree polynomial resulting in the equation

\[
p = A_1 S^2 - A_2 S + A_3
\]  

(2)
in which $A_1 = C_1 + C_2 + C_3$, $A_2 = C_1 (S_1 + S_2) + C_2 (S_o + S_2) + C_3 (S_o + S_1)$ and $A_3 = C_1 S_1 S_2 + C_2 S_o S_2 + C_3 S_o S_1$. The subscripts of the $S$'s denote the values at the three consecutive data points; $S_o$ is the first at the smallest value of pressure, $S_1$ is the second and $S_2$ is the third data point and the $C$'s are defined in turn by

\[
C_1 = \frac{P_o}{(S_o - S_1)(S_o - S_2)}, \quad C_2 = \frac{P_1}{(S_1 - S_o)(S_1 - S_2)}
\]

\[
C_3 = \frac{P_2}{(S_2 - S_o)(S_2 - S_1)}
\]

in which $P_o$, $P_1$, and $P_2$ are the values for pressures at the three consecutive data points corresponding to the saturation values $S_o$, $S_1$, and $S_2$ respectively.

Values for $S$ are obtained by solving Equation 2 with the quadratic formula giving

\[
S = \frac{A_2 - \sqrt{A_2^2 + 4A_1 (A_3 - p)}}{2A_1}
\]

(Note that the negative sign is used preceding the square root).

Values for the partial derivative of $S$ with respect to $p$ are obtained by differentiating Equation 2, giving
Values for $K_r$ corresponding to each of the specified equally incremented pressures are obtained by evaluating the Burdine integral, Equation 1.

Substituting from Equation 2 for the pressure gives the equation shown below

\[
\frac{dS}{dp} \frac{dS}{dp} = \frac{1}{2 A_1 S - A_2} \quad (5)
\]

\[
\int_{S_1}^{S_2} \frac{dS}{S^2} = \int_{S_1}^{S_2} \frac{dS}{\left[ A_1 S^2 - A_2 S + A_3 \right]^2} = \left[ \frac{2 A_1 S - A_2}{8p} \right]
\]

\[
+ \frac{4A_1}{q^{3/2}} \tan^{-1} \left[ \frac{2 A_1 S - A_2}{q^{1/2}} \right] \bigg|_{S_1}^{S_2} \quad (6)
\]

in which $q = 4A_1 A_3 - A_2^2$ and $S_1$ and $S_2$ are the values of saturation at the beginning and end of increment. $S_1$ is larger in value than $S_2$.

After carrying out this integration for each of the specified increments, it is necessary to evaluate the remaining increment of the integral from the smallest value of saturation given in the input data to the saturation equal to the residual saturation $S_r$. This incremental integration is accomplished by assuming that the effective saturation-pressure relation over this range of saturation plots as a straight line on log-log paper, i.e., $S_e = (p_b/p)^\lambda$ in

\[-6-\]
which $p_b$ is the bubbling pressure as defined in the references cited earlier, and $\lambda$ is the slope of the line on log-log paper and has been referred to as the grain size distribution coefficient.

This remaining increment is given by

$$- \int_{S_r}^{S_s} \frac{dS}{p^2} = \frac{\lambda}{p_b^2} \frac{(S_s - S_r)^{2/\lambda+1}}{(1 - S_r)^{2/\lambda}}$$

in which $S_s$ is the smallest value of saturation given in the input data. Justification for the assumption that $S_e$ plots against $p$ as a straight line on log-log paper, particularly in this interval of pressure, is given by Brooks and Corey (1964) and is substantiated by White's (1970) more recent work.

The integrals accumulated at each integration step are stored temporarily in the computer's core memory. The final accumulated integral which is obtained by adding the value from Equation 7 to the previously accumulated integrals from Equation 6 equals the value of the integral in the denominator of Equation 1. Let this accumulated amount be denoted by $T$, that is

$$T = \int_{S_r}^{1} \frac{dS}{p^2}$$
and the temporarily stored values of the accumulated integral be
denoted by t(I) in which I = 1, 2..., number of specified incre-
ments such that t(I) corresponds to the largest values of the input
saturation and pressure data, and t(N) corresponds to the smallest
of these values. Values for K_r, corresponding to the N equal
increments of pressure are subsequently obtained by

\[ K_r(I) = \left( \frac{S(I) - S_r}{1 - S_r} \right)^2 t(N+1 - I)/T \]  

Values for the partial derivative of the relative permeability
with respect to the pressure are obtained by noting that

\[ \frac{\partial K_r}{\partial p} = \frac{dK_r}{dp} = \frac{dK_r}{dS_e} \cdot \frac{dS_e}{dS} \cdot \frac{dS}{dp} \]  

in which S_e as defined previously is the effective saturation, i.e.
\[ S_e = (S - S_r)/(1 - S_r) \] and \[ dS_e/dS = 1/(1 - S_r) \]. Values for dS/dp have
already been obtained from Equation 5. Values for the derivative
dK_r/dS_e are given by

\[ \frac{dK_r}{dS_e}(I) = \frac{1}{T} S_e^2(I) \frac{1-S_r}{p^2(I)} + 2 S_e(I) t(N+1 - I) \]  

The stored values from Equations 5, 9, and 11 permit values for
\( \frac{1}{K_r} \left( \frac{\partial K_r}{\partial p_h} \right) \) and \( \frac{1}{K_r} \left( \frac{\partial S}{\partial p_h} \right) \) to be computed for each of the \( N \) equal increments of capillary pressure referred to earlier.
The names of the FORTRAN variables which are required as input to the computer program are listed in the first column of Table 1. The first card shown in this table contains all the control variables. The columns of the card into which the values of these variables are to be punched are shown in the third column of Table 1, and a description of the significance of each variable is contained in the last column of the table. Subsequent cards, as many in number as required, contain the saturation capillary pressure head data which is used in the evaluation of the Burdine Integrals.

A listing of the output from the program is given in Table 2. This output resulted from execution of the program using the data contained at the end of the listing of FORTRAN statements in Figure 1.
Table 1. Data required as input to the FORTRAN program

<table>
<thead>
<tr>
<th>FORTRAN variable name</th>
<th>Card no.</th>
<th>Columns (right justif.)</th>
<th>Description of Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>1</td>
<td>1-5</td>
<td>An integer variable which specifies the number of data points of saturation and pressure head data which are to be read subsequently.</td>
</tr>
<tr>
<td>NFT</td>
<td>1</td>
<td>6-10</td>
<td>An integer variable which specifies whether the input pressure head data is in units of feet or centimeters. If in feet NFT = 0. If in centimeter NFT&gt;0.</td>
</tr>
<tr>
<td>NINC</td>
<td>1</td>
<td>11-15</td>
<td>An integer variable which specifies the number of increments at which the various quantities are to be printed. The increment of pressure between consecutively printed values will be one-half as large for the first portion of the table as for the last portion of the table.</td>
</tr>
<tr>
<td>AMBDA</td>
<td>1</td>
<td>16-25</td>
<td>A real variable whose magnitude equals the pore size distribution exponent ( \lambda ) referred to in the literature. Its magnitude is determined as the slope of the capillary pressure effective saturation data for smaller values of saturation when plotted on log-log graph paper.</td>
</tr>
<tr>
<td>SR</td>
<td>1</td>
<td>26-35</td>
<td>A real variable whose magnitude equals the residual saturation. The residual saturation may be interpreted physically as the saturation at which moisture movement ceases, but its value is generally determined to get as</td>
</tr>
</tbody>
</table>
Table 1, Continued

<table>
<thead>
<tr>
<th>FORTRAN variable name</th>
<th>Card no.</th>
<th>Columns (right justif.)</th>
<th>Description of Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>array across entire card with 8F10.5</td>
<td>good a fit as possible of data for effective saturation versus pressure to a straight line on a log-log plot (see Brooks and Corey, 1964).</td>
</tr>
<tr>
<td>PB</td>
<td>1</td>
<td>36-45</td>
<td>A real variable whose magnitude equals the bubbling pressure head. The magnitude of the bubbling pressure, as defined by Brooks and Corey, 1964, is the pressure at unit saturation given by a straight line on log-log paper through data for effective saturation versus pressure.</td>
</tr>
<tr>
<td>PO</td>
<td>1</td>
<td>46-55</td>
<td>A real variable whose magnitude equals the actual pressure head at which the saturation first begins to decrease from unity. Its magnitude is generally less in absolute value than the bubbling pressure head.</td>
</tr>
<tr>
<td>PC(I) and S(I)</td>
<td>2</td>
<td>array across entire card with 8F10.5</td>
<td>The array PC represents the capillary pressure head and is given in terms of positive values. S(I) is an array representing the saturation, with magnitudes equal to unity or less. This data is punched such that the saturation corresponding to each pressure head follows the pressure head data immediately. The first values are for the smaller pressure heads (largest values of saturation) and the final values are for the larger values of pressure (smaller values of saturation).</td>
</tr>
</tbody>
</table>
Figure 1. Listing of FORTRAN statement which constitutes the program for obtaining the relative permeability from saturation capillary pressure data.

```
@FORTRAN
REAL RK(100), SAT(100), R(100), OSP(100), DKP(100), PC(60), S(60)
READ (5,101) N,NFT,NINC,AMBDA,SR,PB,PO
IF (N.GT. 60) STOP
100 FORMAT (3IS,4F10.5)
C PO IS THE PRESSURE AT UNIT SATURATION
WRITE(6,102) AMBDA,SR,PB,PO
102 FORMAT (9AMBDA=',F3.3,' SR=',F8.4,' PB=',F8.3,' PO=',F8.4)
UNITY = -1.0
N1=N-1
READ (5,101) (PC(I),S(I),I=1,N)
101 FORMAT (8F10.5)
IF (NFT.GT. 0) GO TO 12
FTCM=1.0/30.4801
DO 13 I=1,N
13 PC(I)=FTCM*PC(I)
12 I1=1
WRITE(6,107) (I,PC(I),S(I),I=1,N)
107 FORMAT (1CAPILLARY TENSION AND SATURATION INPUT DATA*,10(/*1H.*3($13,2F10.5)))
I2=2
I3=3
NC3=NINC/3
NCB=2*NC3
NCF=NINC-NCB
DELT1=(PC(N)-PC(I1))/FLOAT(NCB+2*(NCF-1))
DELT2=2.*DELT1
NCBP=NCB+1
SRM1=1.0-SR
ALPHA=3.*AMBDA+2.*
P=PC(I)
SUM1=0.0
C1=PC(I1)/((S(I1)-S(I2))*S(I1)-S(I3))
C2=PC(I2)/((S(I2)-S(I1))*S(I2)-S(I3))
C3=PC(I3)/((S(I3)-S(I1))*S(I3)-S(I2))
C=C1+C2+C3
```
Figure 1, Continued

\[ C_{5} = 2 \times C \]
\[ C_{CC} = C_{1} \times (S(I2) + S(I3)) + C_{2} \times (S(I1) + S(I3)) + C_{3} \times (S(I1) + S(I2)) \]
\[ A = C_{1} \times S(I2) \times S(I3) \times C_{2} \times S(I1) \times S(I3) \times C_{3} \times S(I1) \times S(I2) \]
\[ B = -C_{CC} \]
\[ SAT_{1} = 1.0 \]
\[ DELTAP = DELT1 \]
\[ DO 1 \ I = 1 + NINC \]

IF \( P \cdot LT. \ PC(I2) \cdot OR. \ I2 \cdot EQ. \ N1 \) GO TO 3

2

\[ I1 = I1 + 1 \]
\[ I2 = I2 + 1 \]
\[ I3 = I3 + 1 \]

IF \( P \cdot GT. \ PC(I2) \cdot AND. \ I2 \cdot LT. \ N1 \) GO TO 2

\[ C_{1} = PC(I1) / ((S(I1) - S(I2)) \times (S(I1) - S(I3))) \]
\[ C_{2} = PC(I2) / ((S(I2) - S(I1)) \times (S(I2) - S(I3))) \]
\[ C_{3} = PC(I3) / ((S(I3) - S(I1)) \times (S(I3) - S(I2))) \]

\[ C = C_{1} \times C_{2} \times C_{3} \]
\[ C_{5} = 2 \times C \]
\[ C_{CC} = C_{1} \times (S(I2) + S(I3)) + C_{2} \times (S(I1) + S(I3)) + C_{3} \times (S(I1) + S(I2)) \]

\[ A = C_{1} \times S(I2) \times S(I3) \times C_{2} \times S(I1) \times S(I3) \times C_{3} \times S(I1) \times S(I2) \]

\[ B = -C_{CC} \]

3

IF \( I \cdot EQ. \ NCBP \) DELTAP = DELT2

\[ P2 = P \cdot GT. \ DELTAP \]
\[ BB4A = B \times 8 - 4 \times (A - P) \times C \]
\[ SBB4A = DSQR1(BB4A) \]
\[ SAT2 = (CCC \times SBB4A) / (2 \times C) \]
\[ SAT2Z = CCC \times SBB4A / (2 \times C) \]
\[ SLT22 = S(I2) \times (S(I1) - S(I2)) \times (P - PC(I2)) / (PC(I1) - PC(I2)) \]

IF \( (ABS(SAT22 - SLT22)) \cdot LT. \ ABS(SAT2 - SLT22) \) SAT2 = SAT22

\[ RL1 = (SAT2 - SRM1) / SRM1 \]
\[ Q = 4. \times A \times C - B \times B \]
\[ SM = C5 \times SAT1 \times B \]
\[ SM = C5 \times SAT2 \times B \]
\[ SAT(I) = SAT2 \]
\[ DSP(I) = UNITY / SM \]
\[ SQ = SQR1(ABS(SQ)) \]

IF \( I \cdot LT. \ NINC \) GO TO 86
Figure 1, Continued

SE2 = (SAT2 - SRM1)/SRM1
AB2 = (2 * AMBDA)/AMBDA
SPBA = SRM1 / (4 * AB2)
SMI = SPBA * SE1 / AB2
SUM = SPBA * SE2 / AB2
SUM1 = SUM1 + SMI + SUM
RK (I) = SUM1
SUM1 = SUM1 + SUM
GO TO 85

85 SM2 = SM / (Q * P) + 4 * C / (Q * SQO) * ATAN2 (SM * SQO)
SMI = SM0 / (Q * PO) + 4 * C / (Q * SQO) * ATAN2 (SM0 * SQO)
SUM1 = SUM1 + ABS (SM1 - SM2)
RK (I) = SUM1
SAT1 = SAT2
PO = P

10 FORMAT (6, 109)
WRITE (6, 109)

109 FORMAT (’NO. PRESSURE SATURATION EFFECT. SAT. RELATIVE K
$DS / DP / KR $DKR / DP / KP’)

P = PC (I)
DELTAP = DELT1
DO 4 I = 1, NINC
RK (I) = SUM1 - RK (I)
RR = R (I)**2
RRK = RR * RK (I) / SUM1
DKSE = (RR * SRM1 / DKP (I) ** 2 + 2 * RK (I) * R (I)) / SUM1
DKP (I) = DSP (I) * DKSE / (SRM1 * RRK)
RK (I) = RRK
DSP (I) = DSP (I) / RRK
WRITE (6, 110) I, P, SAT (I), R (I), RK (I), DSP (I), DKP (I)
IF (I = EQ. NCBP) DELTAP = DELT2
4 P = P + DELTAP

110 FORMAT (1H, ’I3, 3F12.4, 3E13.6)
GO TO 10
END
Figure 1, Continued

<table>
<thead>
<tr>
<th>Ax0t</th>
<th>0</th>
<th>75</th>
<th>1.56</th>
<th>.340</th>
<th>.38</th>
<th>.3275</th>
</tr>
</thead>
<tbody>
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<td>0.9996</td>
<td>20.0</td>
<td>.998</td>
<td>46.0</td>
<td>.995</td>
<td>74.0</td>
</tr>
<tr>
<td>88.0</td>
<td>.990</td>
<td>90.0</td>
<td>.988</td>
<td>92.0</td>
<td>.983</td>
<td>94.0</td>
</tr>
<tr>
<td>96.0</td>
<td>.979</td>
<td>98.0</td>
<td>.976</td>
<td>100.0</td>
<td>.962</td>
<td>101.8</td>
</tr>
<tr>
<td>103.6</td>
<td>.879</td>
<td>105.8</td>
<td>.834</td>
<td>107.8</td>
<td>.789</td>
<td>109.6</td>
</tr>
<tr>
<td>111.8</td>
<td>.727</td>
<td>113.7</td>
<td>.710</td>
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<td>.684</td>
<td>117.9</td>
</tr>
<tr>
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<td>.658</td>
<td>121.5</td>
<td>.648</td>
<td>131.0</td>
<td>.613</td>
<td>141.7</td>
</tr>
<tr>
<td>151.5</td>
<td>.549</td>
<td>161.5</td>
<td>.527</td>
<td>171.4</td>
<td>.511</td>
<td>181.2</td>
</tr>
<tr>
<td>201.5</td>
<td>.468</td>
<td>221.3</td>
<td>.458</td>
<td>243.2</td>
<td>.437</td>
<td>266.6</td>
</tr>
<tr>
<td>299.0</td>
<td>.406</td>
<td>354.8</td>
<td>.387</td>
<td>401.6</td>
<td>.380</td>
<td></td>
</tr>
</tbody>
</table>

aFIN
Table 2. Example of output obtained from the computer program in Figure 1, using the input data contained at the end of this listing.

<table>
<thead>
<tr>
<th>NO.</th>
<th>PRESSURE</th>
<th>SATURATION</th>
<th>EFFECT</th>
<th>SAT.</th>
<th>RELATIVE K</th>
<th>DS/DP/KR</th>
<th>DKR/DP/KR</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.3281</td>
<td>0.9996</td>
<td>0.9994</td>
<td>0.8664263+00</td>
<td>0.652713-02</td>
<td>0.111914+01</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.4592</td>
<td>0.9889</td>
<td>0.9984</td>
<td>0.727955+00</td>
<td>0.683041-02</td>
<td>0.602588+00</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.5903</td>
<td>0.9983</td>
<td>0.9974</td>
<td>0.657479+00</td>
<td>0.683702-02</td>
<td>0.368847+00</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.7214</td>
<td>0.9977</td>
<td>0.9965</td>
<td>0.632795+00</td>
<td>0.780727-02</td>
<td>0.286116+00</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.8525</td>
<td>0.9971</td>
<td>0.9956</td>
<td>0.614285+00</td>
<td>0.668342-02</td>
<td>0.178356+00</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>0.9836</td>
<td>0.9966</td>
<td>0.9948</td>
<td>0.602502+00</td>
<td>0.595445-02</td>
<td>0.121761+00</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>1.1147</td>
<td>0.9961</td>
<td>0.9930</td>
<td>0.594030+00</td>
<td>0.542097-02</td>
<td>0.888232-01</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>1.2458</td>
<td>0.9957</td>
<td>0.9935</td>
<td>0.588040+00</td>
<td>0.502559-02</td>
<td>0.671769-01</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>1.3769</td>
<td>0.9954</td>
<td>0.9930</td>
<td>0.583813+00</td>
<td>0.470144-02</td>
<td>0.528669-01</td>
<td></td>
</tr>
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16 3.59579 0.76700 17 3.66797 0.72700 18 3.73030 0.71000
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28 5.91446 0.48600 29 6.10878 0.48000 30 6.26047 0.48500
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Table 2. Example of output obtained from the computer program in Figure 1, using the input data contained at the end of this listing.
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