APPENDIX - II

DERIVATION OF THE CONSTANTS FOR THE
BEST FITTED STRAIGHT LINE (COMPUTER PROGRAM
USED IN SECTION 4.2)

Given a set of n points \((x_1, f_1), (x_2, f_2), \ldots, (x_n, f_n)\). It is
required to fit a straight line \(N = KS\) i.e. \(\log N = \alpha \log S + \log K\) i.e. \(f(x) = a_0 + a_1x\) through these points. The optimal
values of slope \(a_1\) and intercept \(a_0\) in the above equation for
straight line are to be found. After evaluation of \(a_0\) and \(a_1\), the
value of \(f(x)\) can be calculated for a known values of \(x\). A popular
criterion is to find the value of slope and intercept which
minimises the sum of the square error. In other word, instead of
fitting a polynomial, which exactly reproduces the values of the
function at the sample points we propose to determine a
polynomial function \(\bar{f}(x)\) such that the sum of the square error is
least. This is called the least square fitting. The approximate
\(\bar{f}(x)\) can be written in our case

\[
\bar{f}(x) = a_0 + a_1x
\]

From equation (1)

\[
\begin{align*}
\bar{f}_1 &= a_0 + a_1 x_1 \\
\bar{f}_2 &= a_0 + a_1 x_2 \\
\vdots & \quad \vdots \\
\bar{f}_n &= a_0 + a_1 x_n
\end{align*}
\]

The sum of the square error at the sample points is given by

\[
E(a_0, a_1) = \sum_{j=1}^{n} (f_j - a_0 - a_1 x_j)^2
\]

\[\cdots \ldots (2)\]
E is the function of \(a_0\) and \(a_1\). We wish to determine \(a_0\) and \(a_1\) such that for those values of \(a_0\) and \(a_1\), \(E\) is minimum. The necessary condition for minimum are

\[
\frac{\partial E}{\partial a_0} = \frac{\partial E}{\partial a_1} = 0
\]

The sufficient condition for minimum are

\[
\frac{\partial^2 E}{\partial a_0^2} > 0 \quad \text{also} \quad \frac{\partial^2 E}{\partial a_1^2} > 0
\]

According to the first condition

\[
\frac{\partial E}{\partial a_0} = \sum_{j=1}^{n} 2(f_j - a_0 - a_1x_j)(-1) = 0
\]

or

\[
\sum_{j=1}^{n} (f_j - a_0 - a_1x_j) = 0
\]

i.e.

\[
a_0 \sum_{j=1}^{n} 1 + a_1 \sum_{j=1}^{n} x_j = \sum_{j=1}^{n} f_j
\]

i.e.

\[
a_0 s_0 + a_1 s_1 = T_0
\]

Similarly from equation (2)

\[
\frac{\partial E}{\partial a_1} = \sum_{j=1}^{n} 2(f_j - a_0 - a_1x_j)(-x_j) = 0
\]

i.e.

\[
a_0 \sum_{j=1}^{n} x_j + a_1 \sum_{j=1}^{n} x_j^2 = \sum_{j=1}^{n} f_j x_j
\]

\[
a_0 s_1 + a_1 s_2 = T_1
\]

Solving equations (3) and (4)

\[
a_0 s_0 s_2 + a_1 s_1 s_2 = T_0 s_2
\]

\[
a_0 s_1^2 + a_1 s_1 s_2 = T_1 s_1
\]
Subtracting

\[ a_0(S_0S_2 - S_1^2) = T_0S_2 - T_1S_1 \]

\[ a_0 = - \frac{T_0S_2 - T_1S_1}{S_1^2 - S_0S_2} \quad \ldots \quad (5) \]

Similarly

\[ a_0S_1S_0 + a_1S_1^2 = T_0S_1 \]

Also \[ a_0S_1S_0 + a_1S_1S_2 = T_1S_0 \]

Subtracting

\[ a_1(S_1^2 - S_0S_2) = T_0S_1 - T_1S_0 \]

Thus \[ a_1 = - \frac{T_0S_1 - T_1S_0}{S_1^2 - S_0S_2} \quad \ldots \quad (6) \]

The values of the parameter of equation (5) and (6) are as follows

\[ S_0 = \sum_{j=1}^{n} x_j \quad ; \quad S_1 = \sum_{j=1}^{n} x_j \quad ; \quad T_0 = \sum_{j=1}^{n} f_j \]

\[ S_2 = \sum_{j=1}^{n} x_j^2 \quad ; \quad T_1 = \sum_{j=1}^{n} f_j x_j \]

Substituting the values of constant in equation (6), the slope of equation (6) is

\[
 a_1 = - \frac{T_1S_0 - T_0S_1}{S_0S_2 - S_1^2} \\
 = \frac{n \sum_{j=1}^{n} f_j x_j - \sum_{j=1}^{n} f_j \sum_{j=1}^{n} x_j}{n \sum_{j=1}^{n} x_j^2 - \left( \sum_{j=1}^{n} x_j \right)^2}
\]
If we consider \( N = K S^\alpha \),

In this case \( f_j = \log N_j; \quad a_0 = \log K; \quad a_1 = \alpha \) and \( X = \log S \). Then

\[
\text{Exponent (}\alpha\text{)} = (a_1) = \frac{\sum_{j=1}^{n} \log N_j \log S_j - \sum_{j=1}^{n} \log N_j \sum_{j=1}^{n} \log S_j}{\sum_{j=1}^{n} (\log S_j)^2 - \left( \sum_{j=1}^{n} \log S_j \right)^2} \quad \ldots \quad (7)
\]

Equation (7) is used to determine the exponent \( \alpha \) of the equation \( N = K S^\alpha \). The computer programme along with the result is attached separately in this thesis for a particular data set obtained from the T.D.C. Similarly substituting the values of parameters in equation (5)

\[
a_0 = \frac{S_0 T S_1 - T_0 S_2}{S_2 - S_0 S_2} = \frac{\sum_{j=1}^{n} f_j x_j - \sum_{j=1}^{n} f_j \sum_{j=1}^{n} x_j}{\left( \sum_{j=1}^{n} x_j \right)^2 - n \sum_{j=1}^{n} x_j^2}
\]

The values of \( a_0 \) can be written directly from equation (3)

\[
\log K = a_0 = \frac{1}{n} \left[ \sum_{j=1}^{n} f_j - a_1 \sum_{j=1}^{n} x_j \right]
\]

\[\text{i.e.} \quad K = \frac{1}{n} \left[ \sum_{j=1}^{n} \log N_j - \alpha \sum_{j=1}^{n} \log S_j \right] \quad \ldots \quad (8)
\]

The equation (8) is used to determine the constant \( K \) of the equation \( N = K S^\alpha \) of the best fitted straight line. The detail printout (including the computer programme) of the I.B.M. 1620 computer is also attached in this thesis.
FITTING A STRAIGHT LINE

DIMENSION S(4), P(4), E(4), F(4), SLOPE(2), VINT(2), CCN05(2), CCN1(2), IE RMS(2)

N = 4
AN = N
DO 15 JJ = 1, 2
READ 1, SUME, SUMSE, SUMF, SUMFE, ERROR, (S(I) * I = 1, N), (P(I) * I = 1, N)

1 FORMAT(13F6.2)
DO 5 K = 1, 4
E(K) = (LOG(S(K))) * 0.4343
F(K) = (LOG(P(K))) * 0.4343

DO 10 I = 1, N
SUME = SUME + E(I)
SUMSE = SUMSE + E(I) * E(I)
SUMF = SUMF + F(I)
10 SUMFE = SUMFE + F(I) * E(I)

SLOPE(JJ) = (AN * SUMFE - SUME * SUMF) / (AN * SUMSE - SUME * SUME)
VINT(JJ) = 10.0 ** ((SUMF - SLOPE(JJ) * SUME) / AN)
CCN05(JJ) = VINT(JJ) * (0.5 ** SLOPE(JJ))
CCN1(JJ) = VINT(JJ) * (1.0 ** SLOPE(JJ))

DO 50 I = 1, N
50 ERROR = ERROR + (P(I) - VINT(JJ) * (S(I) ** SLOPE(JJ))) ** 2
15 ERMS(JJ) = SQRT(ERROR / AN)

PRINT 25, (SLOPE(I), I = 1, 2), (VINT(I), I = 1, 2), (CCN05(I), I = 1, 2), (CCN1(I), I = 1, 2), (ERMS(I), I = 1, 2)

25 FORMAT(5X, 5H SLOPE =, 2(5X, F8.3)/5X, 5HVINT =, 2(5X, F8.3)/5X, 5HCCN05 =, 2(5X, F8.3)/5X, 5HCCN1 =, 2(5X, F8.3)/5X, 5HERMS =, 2(5X, F8.3))

STOP
END
### Appendix II

#### I) Computation of Constants K and \( \alpha \) of the eqn

<table>
<thead>
<tr>
<th>( K )</th>
<th>( \alpha )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.207</td>
<td>10.05</td>
</tr>
<tr>
<td>0.809</td>
<td>5.92</td>
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</table>

#### II) Comparison of data of supersaturation spectra with other workers

<table>
<thead>
<tr>
<th>N</th>
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<th>( \alpha )</th>
</tr>
</thead>
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<tr>
<td>100</td>
<td>1.54</td>
<td>9.52</td>
</tr>
<tr>
<td>0.9</td>
<td>1.22</td>
<td>7.34</td>
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<tr>
<td>0.7</td>
<td>1.01</td>
<td>6.12</td>
</tr>
<tr>
<td>0.5</td>
<td>0.80</td>
<td>5.00</td>
</tr>
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<tr>
<td>0.5</td>
<td>0.80</td>
<td>5.00</td>
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**Stop**

<table>
<thead>
<tr>
<th>SLOPE</th>
<th>( ERMS )</th>
<th>CCN 05</th>
<th>CCN 1</th>
<th>ERMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.387</td>
<td>106.654</td>
<td>4.278</td>
<td>106.654</td>
<td>12.455</td>
</tr>
<tr>
<td>40.987</td>
<td>106.654</td>
<td>4.278</td>
<td>106.654</td>
<td>12.455</td>
</tr>
</tbody>
</table>

**Stop**
DIMENSION S(6),P(6),SL(OPE(2)),VINT(2),CCN05(2),CCN1(2),IERMS(2) & N=6

READ JJ=1,2 SUME,SUMSE,SUMF,SUMFE,ERROR♦(S(I),I=1,N5,P(I)),I=1,N)

1 FORMAT(11F6.2)

DO K = 1,6 E(K) = (LOG(S(K)))*0.4343 = 5 F K) = {LOG(P(K)))*0.4343

DO 10 I = 1, N SUME = SUME + E(I )

SUMSE = SUMSE + E(I ) * E(I )

SUMF = SUMF + F(I )

SUMFE = SUMFE + F(I ) * E(I )

SLOPE(JJ) = (AN*SUMFE - SUME*SUMF)/(AN*SUMSE - SUME*SUME)

VINT (JJ) = 10.0 ** ( (SUMF - SLOPE(JJ)*SUME)/AN)

CCN05(JJ) = VINT(JJ) * (0.5** SLOPE(JJ))

CCN1(JJ) = VINT(JJ) * (1.0** SLOPE(JJ))

ERROR = ERROR + (P(I ) - VINT(JJ) * (S(I )**SLOPE(JJ)))** 2

ERMS(JJ) = SORTERROR/AN

PRINT 25, (SLOPE(I),I = 1,2), (VINT(I),I = 1,2), (CCN05(I),I = 1,2),

Page 2

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1) **Computation of Constants**

<table>
<thead>
<tr>
<th>$K$ and $N K$ of the eqn</th>
</tr>
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<tbody>
<tr>
<td>165.867</td>
</tr>
<tr>
<td>131.016</td>
</tr>
<tr>
<td>165.867</td>
</tr>
</tbody>
</table>

2) **Result of two data set obtained from T.D.C.**

   | $SLOPE$ | 0.340 |
   | $VINT$  | 165.867 |
   | $CCNO5$ | 131.016 |
   | $CCN1$  | 165.867 |
   | $ERMS$  | 10.282  |
   |         | 16.868  |