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SOME ASPECTS OF THE WATER PACKING PROBLEM

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ABSTRACT

This report is divided into two parts. The first part contains the results of a simulation performed by the two-phase thermohydraulics code Firebird.

The second part of this report deals with the "water packing" problem. Its mathematical and physical interpretations are discussed in detail and a method for identifying a transition node together with an alternate mathematical treatment of the boiling boundary are also included.

ACKNOWLEDGEMENT

I want to express my sincere appreciation to Mr. N. Spinks and Dr. D. Rennick of the thermohydraulics branch of Atomic Energy of Canada Ltd. for their kind assistance throughout all phases of this work.

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CHAPTER 1

CODE VERIFICATION

1.1 Introduction

Firebird is a thermohydraulics simulation code which was developed in the thermohydraulics branch of Atomic Energy of Canada Ltd. in Meadowvale, Ontario. The main features of this code are:

(i) Homogeneous two-phase flow model

(ii) Implicit solution of the equations by the method of porsching

(iii) Derivative smoothing across phase boundaries.

This report outlines the simulation of some experiments using Firebird. These experiments which were scaled down versions of actual reactor networks were performed by Westinghouse Canada Ltd.

Verification of test #592 was first performed by an "old" version of Firebird. This "old" version is a special version of Firebird which was re-arranged by S.M. Chu, of the thermohydraulics branch, to model a single pipe blowdown and emergency core cooling injection. This version retains the essential features of Firebird, e.g.: numerical scheme, properties formulation, derivative smoothing, etc. Results obtained with this version are reported in Section 1.3.2.

Another version of Firebird was then used to simulate the same experiment (#592). This version contained a flow regime indicator and could account for density variation in stratified flow. Results obtained with this version are reported in Section 1.3.3.

1.2 Changes Made to Old Code

The data blocks containing the time variation of the injection pressure and downstream of the break pressure were made identical to those of test #592. These boundary conditions were obtained from computer plots of the actual experimental results. These plots are shown on Figures 1.2.1, 1.2.2 and 1.2.3.

A slightly modification was also made to account for the difference in initial temperature between the top and the bottom pin, in the "old" version mentioned in the previous section the initial temperatures were assumed to be vertically uniform. The vertical variation in temperature was accounted for by specifying the exact initial temperatures of the top and bottom pins and finding the other values by interpolation assuming a linear variation as a function of vertical distance (see Appendix A for listing).

1.3 Results

1.3.1 Plotting Convention

The comparison of the experimental results of test #592 and the results predicted by Firebird are shown on Figures 1.3.1 to 1.3.7. The plotting convention is as follows:

Solid line ≡ Experimental results
Circles ≡ Predictions made by the "old" version of Firebird
Triangles ≡ Predictions made by the "old" version with initial temperature variation
Dots ≡ Predictions made by the newer version of Firebird (with flow regime indicator and allowance for density variation)

TIME PUMP PRESS. DOWN PRESS.

```
UCL HP TRANSITION DATA,RAJAN'S TAPE AEC849,ACCESS DATE       78-05-11 DFRTASF
FILE =   13 TEST NO. 592MS=   0 MSPLOT=   0  DFRHPDX  78-05-11
   0.0 3075.97   95.39 |    .0 3068.41   41.67 |   1.0 3069.36   36.22 |   2.0 3066.52   35.10
   3.8 3069.36   31.71 |   4.8 3067.47   29.84 |   5.8 3068.41   29.45 |   6.8 3063.69   27.96
   7.8 2962.55   26.50 |   8.8 2971.06   22.91 |   9.8 2953.10   23.62 |  10.8 2973.89   24.67
  11.8 2969.17   25.45 |  12.8 2956.88   26.89 |  13.8 2955.93   26.74 |  14.8 2958.77   27.69
  15.8 2955.93   28.46 |  16.8 2972.00   29.62 |  17.8 2975.78   30.50 |  18.8 2989.96   31.48
  19.8 3007.92   32.80 |  20.8 3021.15   33.34 |  21.8 3047.62   34.59 |  22.8 3055.18   35.57
  23.8 3050.45   37.10 |  24.8 3047.62   37.95 |  25.8 3056.13   39.30 |  26.8 3066.52   40.08
  27.8 3074.08   41.43 |  28.8 3088.26   42.45 |  29.8 3089.21   43.30 |  30.8 3092.99   44.15
  31.8 3085.43   45.67 |  32.8 3068.41   46.69 |  33.8 3073.14   47.74 |  34.8 3066.52   47.57
  35.8 3056.13   48.21 |  36.8 3057.07   48.86 |  37.8 3053.29   49.26 |  38.8 3052.34   50.04
  39.8 3040.06   51.03 |  40.8 3035.33   51.71 |  41.8 3041.95   52.42 |  42.8 3041.95   53.20
  43.8 3044.78   52.28 |  44.8 3045.73   53.20 |  45.8 3067.47   49.84 |  46.8 3072.19   47.47
  47.8 3084.48   30.83 |  48.8 3101.49   29.04 |  49.8 3108.11   28.94 |  50.8 3114.73   29.01
  51.8 3127.01   29.07 |  52.8 3115.67   29.24 |  53.8 3101.49   29.31 |  54.8 3080.70   29.28
  55.8 3069.36   29.28 |  56.8 3045.73   29.38 |  57.8 3023.99   29.28 |  58.8 3010.76   29.31
  59.8 3008.87   29.14 |  60.8 3010.76   29.11 |  61.8 3011.70   29.01 |  62.8 3011.70   28.97
  63.8 3019.26   28.94 |  64.8 3018.32   29.01 |  65.8 3039.11   28.94 |  66.8 3058.96   29.01
  67.8 3059.91   29.01 |  68.8 3067.47   29.07 |  69.8 3069.36   29.14 |  70.8 3067.47   29.18
  71.8 3070.30   29.28 |  72.8 3061.80   29.24 |  73.8 3062.74   29.38 |  74.8 3056.13   29.34
  75.8 3053.29   29.41 |  76.8 3045.73   29.48 |  77.8 3053.29   29.51 |  78.8 3047.62   29.55
  79.8 3050.45   29.58 |  80.8 3043.84   29.72 |  81.8 3054.23   29.68 |  82.8 3058.02   29.72
  83.8 3059.91   29.75 |  84.8 3069.36   29.85 |  85.8 3072.19   29.75 |  86.8 3068.41   29.82
  87.8 3072.19   29.89 |  88.8 3068.41   29.95 |  89.8 3063.69   29.92 |  90.8 3064.63   30.02
  91.8 3061.80   30.02 |  92.8 3066.52   30.09 |  93.8 3056.13   30.16 |  94.8 3058.02   30.19
  95.8 3065.58   30.16 |  96.8 3075.03   30.26 |  97.8 3067.47   30.22 |  98.8 3068.41   30.29
  99.8 3075.97   30.22 | 100.8 3078.81   30.36 | 101.8 3076.92   30.26 | 102.8 3085.43   30.33
 103.8 3088.26   30.36 | 104.8 3075.97   30.39 | 105.8 3075.03   30.36 | 106.8 3082.59   30.39
 107.8 3079.76   30.43 | 108.8 3073.14   30.36 | 109.8 3076.92   30.43 | 110.8 3078.81   30.46
 111.8 3076.92   30.39 | 112.8 3077.86   30.46 | 113.8 3078.81   30.46 | 114.8 3068.41   30.50
 115.8 3065.58   30.46 | 116.8 3055.18   30.50 | 117.8 3046.67   30.50 | 118.9 3039.11   30.53
 120.9 3029.66   30.29 | 122.9 3023.99   29.82 | 124.9 3030.60   29.82 | 126.9 3038.17   29.31
 128.9 3043.84   28.97 | 130.9 3039.11   29.04 | 132.9 3041.00   25.52 | 134.9 3044.78   25.72
 136.9 3046.67   25.93 | 138.9 3049.51   25.82 | 140.9 3045.73   27.48 | 142.9 3043.84   31.78
 144.9 3043.84   37.81 | 146.9 3052.34   47.54 | 148.9 3055.18   56.76 | 150.9 3056.13   71.42
 152.9 3064.63   93.79 | 154.9 3062.74  110.47 | 156.9 3054.23  103.08 | 158.9 3050.45  114.25
 160.9 3064.63  118.13 | 162.9 3065.58  126.66 | 164.9 3083.54  129.62 | 166.9 3089.21  141.16
 168.9 3094.88  126.42 | 170.9 3088.26  142.97 | 172.9 3090.15  167.65 | 174.9 3090.15  203.07
 176.9 3090.15  174.73 | 178.9 3087.32  195.49 | 180.9 3085.43  214.39 | 182.9 3090.15  268.54
 184.9 3082.59  272.33 | 186.9 3090.15  281.44 | 188.9 3087.32  273.81 | 190.9 3092.99  279.44
 192.9 3092.99  269.19 | 194.9 3083.54  260.82 | 196.9 3076.92  266.13 | 198.9 3079.76  265.44
 200.9 3080.70  255.31 | 202.9 3084.48  253.45   204.9 3083.54  253.59 | 206.9 3075.97  247.36
 208.9 3086.37  249.77 | 210.9 3089.21  289.24   212.9 3099.60  286.61 | 214.9 3099.60  278.19
 216.9 3099.60  272.06 | 218.9 3092.99  261.16 | 220.9 3085.43  267.81 | 222.9 3085.43  250.59
 224.9 3077.86  257.41 | 226.9 3080.70  246.36 | 228.9 3073.14  231.50 | 230.9 3079.76  238.65
 232.9 3075.03  229.92 | 234.9 3078.81  221.95 | 236.9 3078.81  208.73 | 238.9 3078.81  216.55
 240.9 3081.65  213.64 | 242.9 3079.76  201.83 | 244.9 3079.76  202.35 | 246.9 3078.81  205.78
 248.9 3083.54  196.41 | 250.9 3074.08  194.87 | 252.9 3078.81  196.21 | 254.9 3078.81  188.50
 256.9 3072.19  190.52 | 258.9 3076.92  179.28 | 260.9 3078.81  182.36 | 262.9 3087.32  172.57
 264.9 3080.70  174.93 | 266.9 3074.08  169.12 | 268.9 3075.97  160.77 | 270.9 3075.97  168.47

  MFB   CRNL MOS/BE 1.1 V01RELEASE434 78-05-05
12.24.52.SIO. 4P     CRNL MOS/BE 1.1 V01RELEASE434 R.C 08.25
BBU24.54.DFRHPDX  FROM SIO/4P FOR CCC
12.24.54.IP  00001024 WORDS - FILE INPUT   , DC 00
12.24.54.DFRHPX8,BB05-91R/60000,T66,I030,CM174000
12.24.54..   --    REMNICK,D.F..  566 --
12.25.10.SENDTO,BP.
parity error received
ROUTE,TP
```

TABLE 1.2.1 TABULATED VALUES OF INJECTION PRESSURE AND DOWNSTREAM OF BREAK PRESSURE.

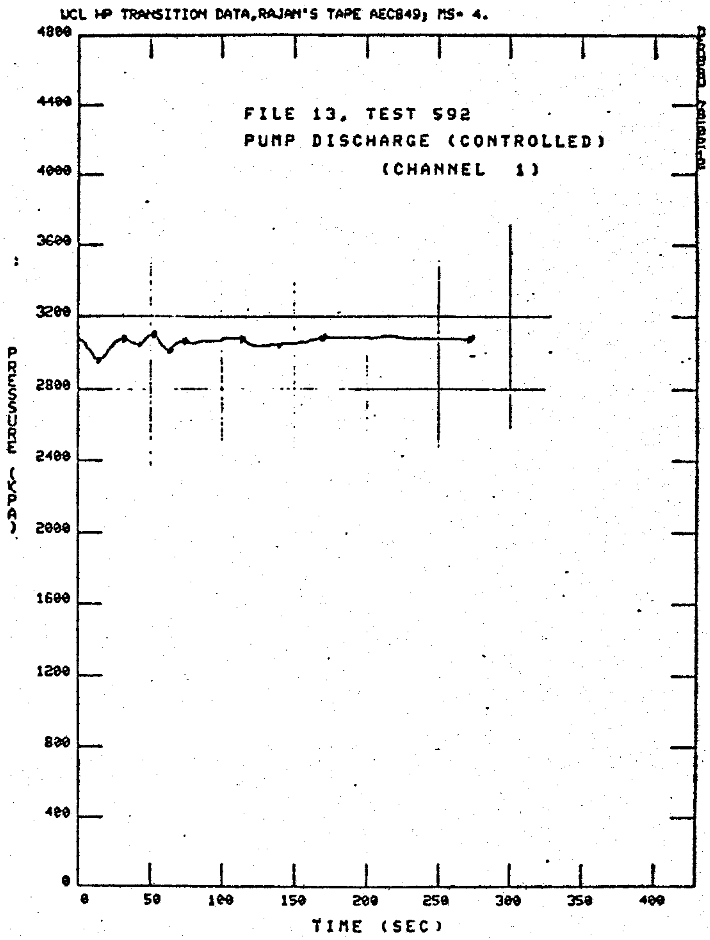


FiG. 1.2.1 Pump Discharge Pressure

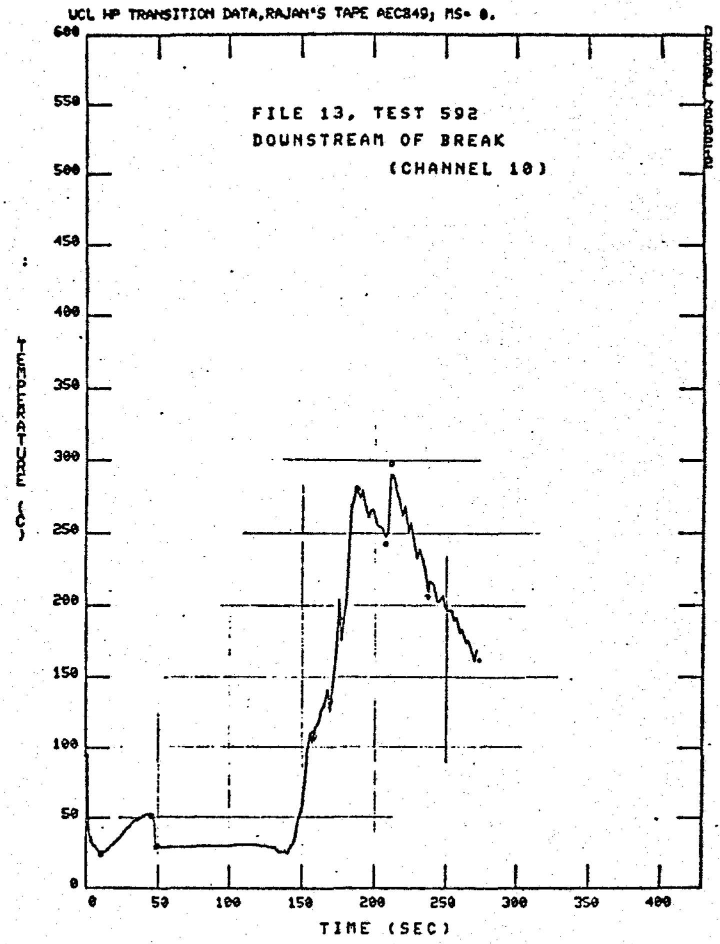


FiG. 1.2.2 DOWNSTREAM OF BREAK PRESSURE

1.3.2 The Old Version

As can be seen in Figures 1.3.1 to 1.3.6 agreement between experimental data and predictions are generally very good, however the following discrepancies are noteworthy:

(i) The code seems to have over predicted the rewetting time for the bottom pins and underpredicted for the top ones in the heated section.

(ii) The outlet header axis temperature was also overpredicted up to about 100 secs, but there was good agreement after that.

Aside from the points mentioned above there was excellent agreement betweeen the experimental results and the predictions made by this "old" version of Firebird.

1.3.3 The Modified Version

The results obtained with this version of Firebird do not differ very much from those obtained with the old version. The mispredictions here are the same as the ones reported on section 1.3.2, and again aside from these discrepancies there was excellent agreement between the experimental results and the predictions made by this modified version of Firebird.

1.4 Conclusion

The thermohydraulics simulation code Firebird has been successfully used to simulate the single channel-single ended cold water injection test #592 performed by Westinghouse Canada Limited.

The overall agreement between the code predictions and the experimental results were generally excellent.

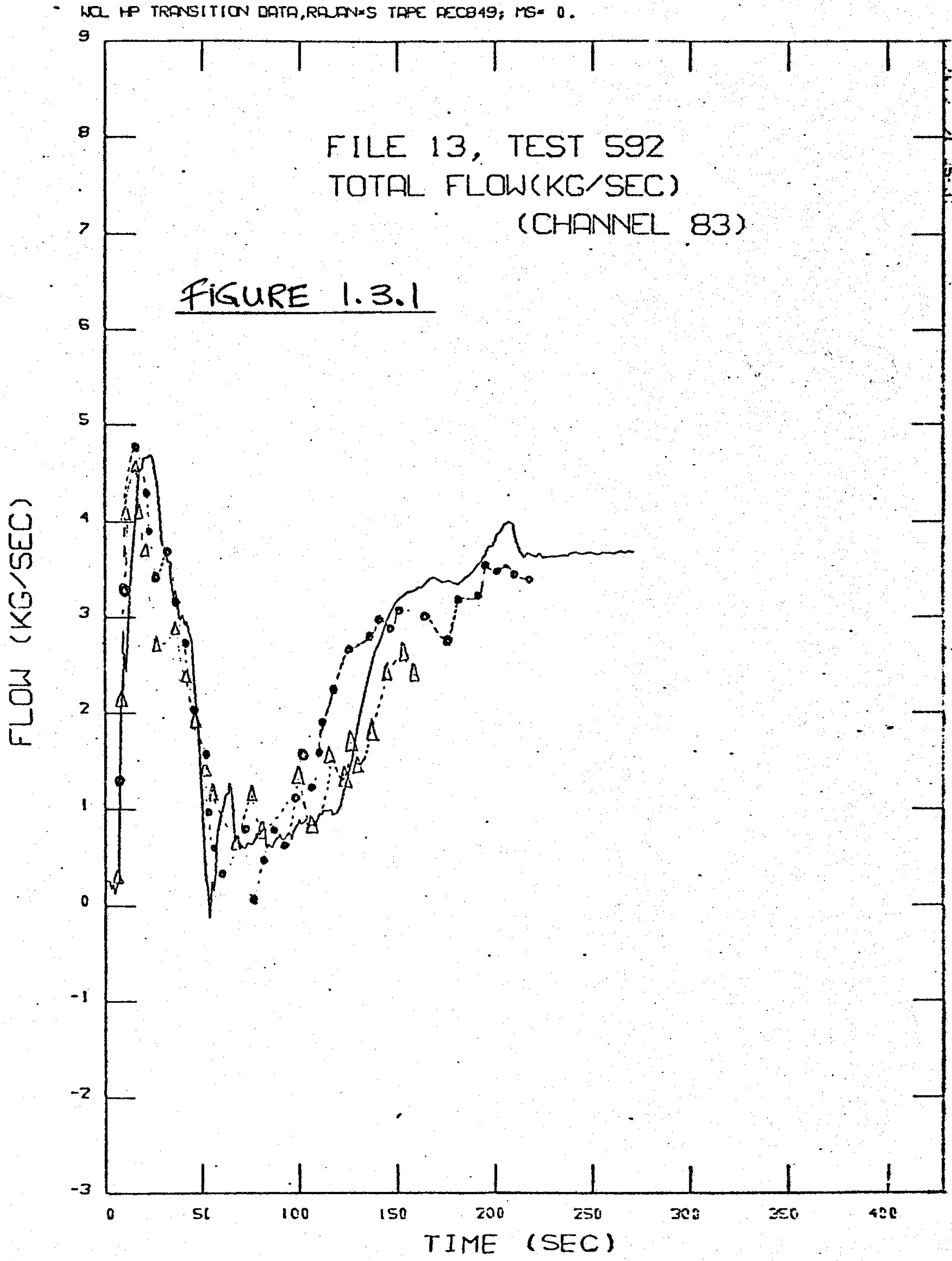

WCL HP TRANSITION DATA,RAJAN=S TAPE REC849; MS= 0.
FILE 13, TEST 592
TOTAL FLOW(KG/SEC)
(CHANNEL 83)
FLOW (KG/SEC)
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
0
50
100
150
200
250
300
350
400
TIME (SEC)

FIGURE 1.3.1

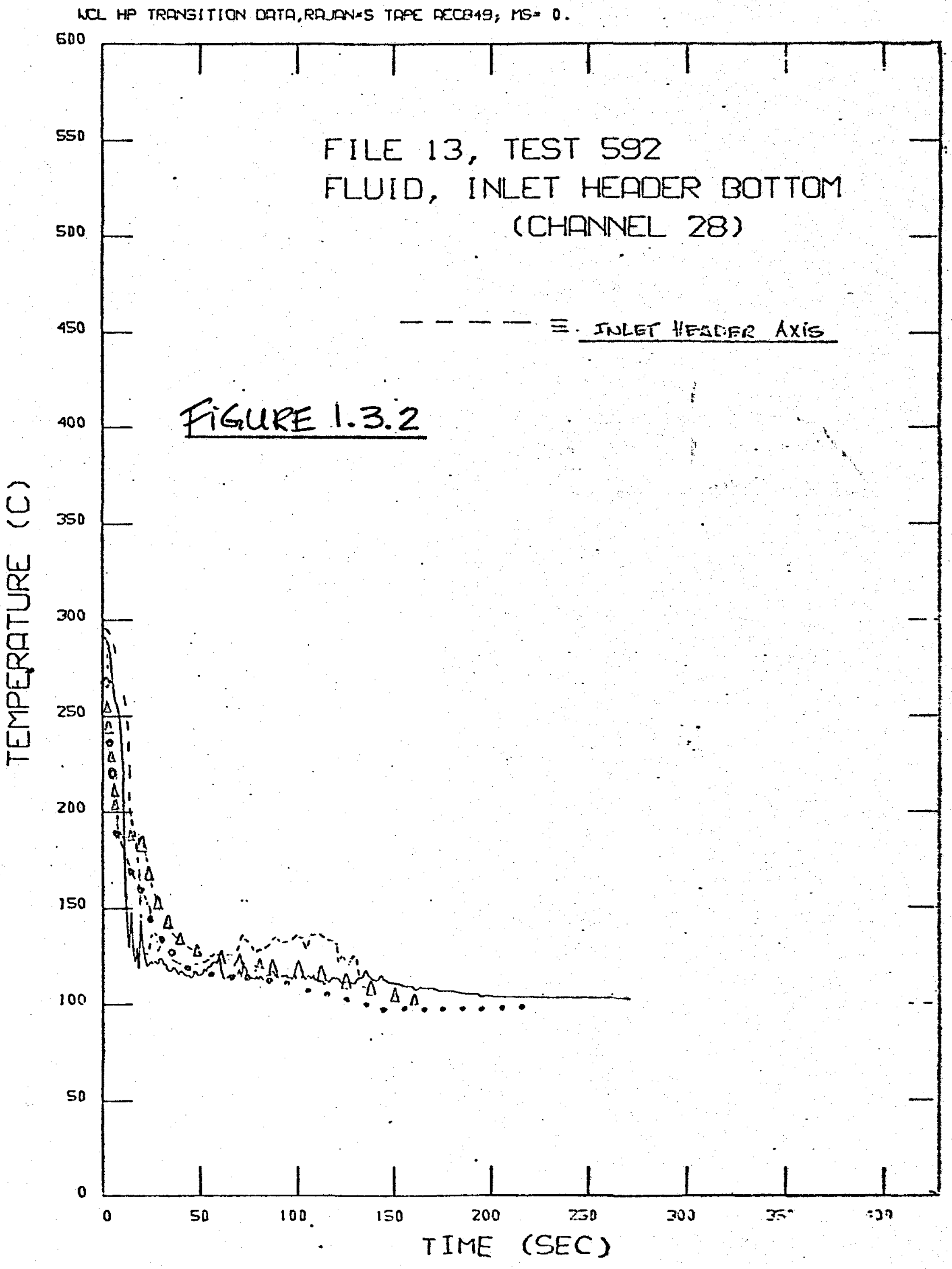

WCL HP TRANSITION DATA,RAJAN=S TAPE REC849; MS= 0.
FILE 13, TEST 592
FLUID, INLET HEADER BOTTOM
(CHANNEL 28)
– – – – ≡ INLET HEADER AXIS
TEMPERATURE (C)
0
50
100
150
200
250
300
350
400
450
500
550
600
TIME (SEC)
0
50
100
150
200
250
300
350
400

FIGURE 1.3.2

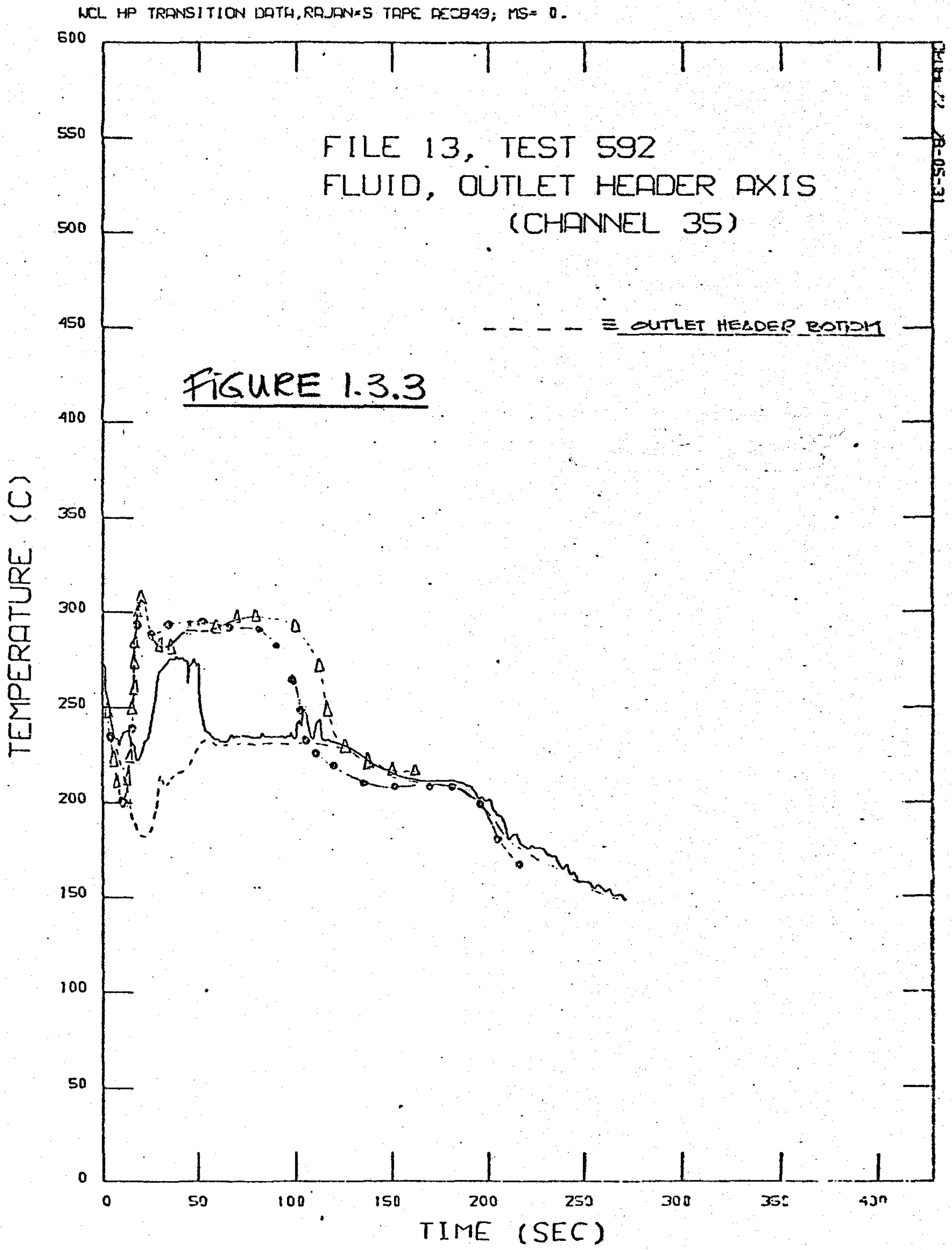

WCL HP TRANSITION DATA,RAJAN*S TAPE AEC849; MS= 0.
FILE 13, TEST 592
FLUID, OUTLET HEADER AXIS
(CHANNEL 35)
- - - - ≡ OUTLET HEADER BOTTOM
78-05-31
TEMPERATURE (C)
600
550
500
450
400
350
300
250
200
150
100
50
0
TIME (SEC)
0
50
100
150
200
250
300
350
400

FIGURE 1.3.3

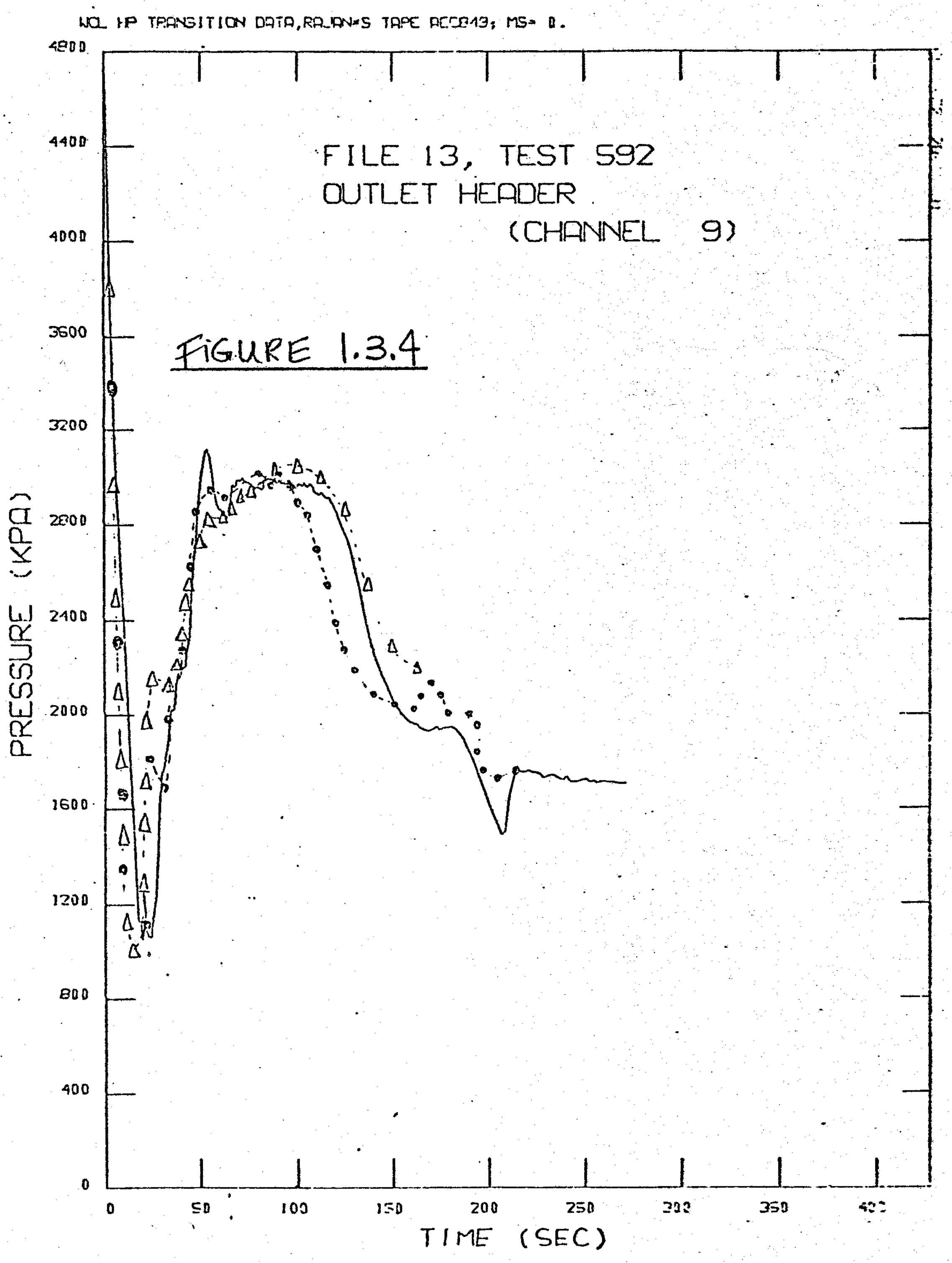

WOL HP TRANSITION DATA,RAJAN*S TAPE ACC843; MS= 0.
FILE 13, TEST 592
OUTLET HEADER
(CHANNEL 9)
PRESSURE (KPA)
4800
4400
4000
3600
3200
2800
2400
2000
1600
1200
800
400
0
0
50
100
150
200
250
300
350
400
TIME (SEC)

FIGURE 1.3.4

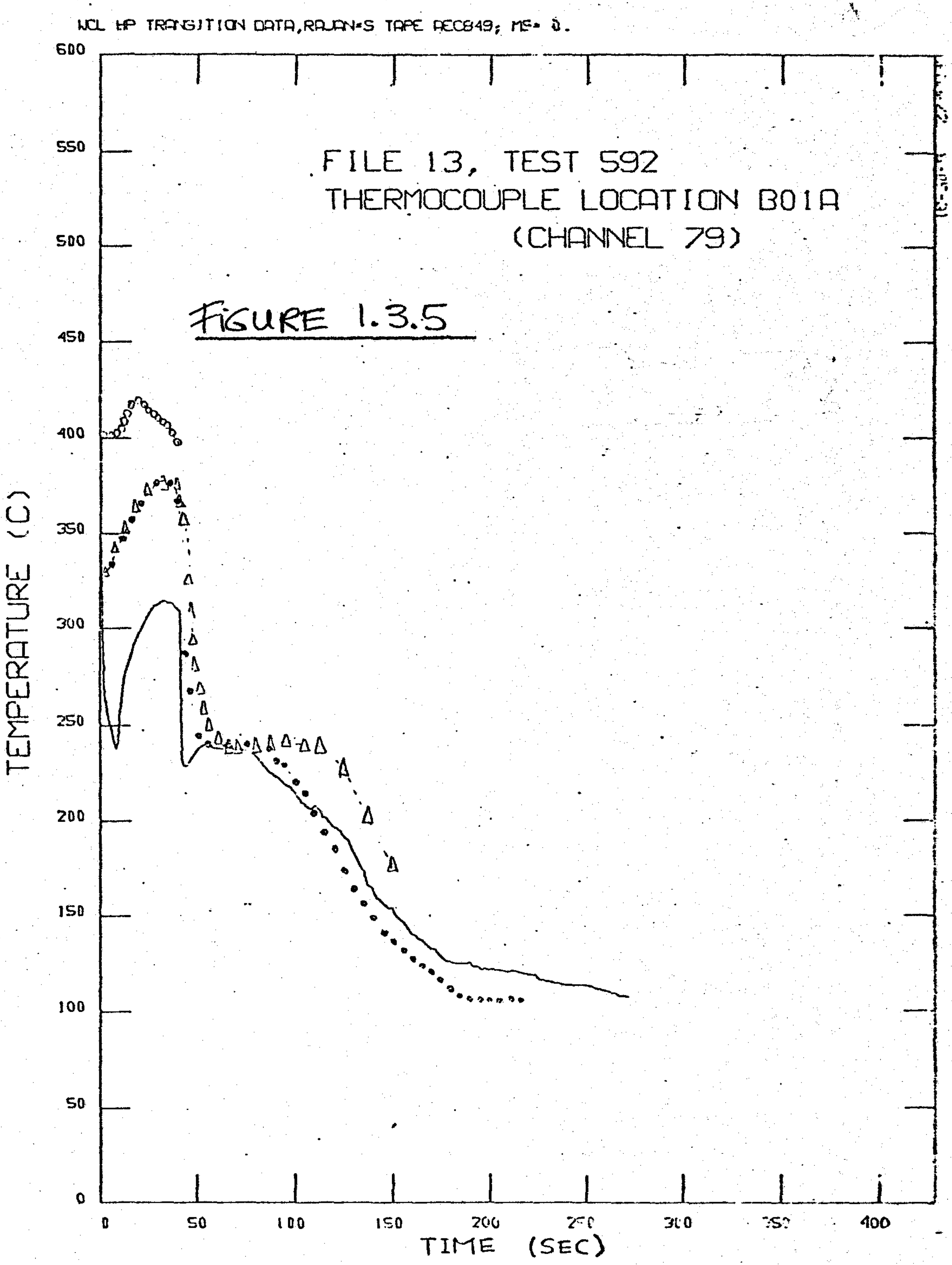


FIGURE 1.3.5

NCL HP TRANSITION DATA,RAJAN'S TAPE REC849; MS= 0.
FILE 13, TEST 592
THERMOCOUPLE LOCATION B01A
(CHANNEL 79)
TEMPERATURE (C)
600
550
500
450
400
350
300
250
200
150
100
50
0
0
50
100
150
200
250
300
350
400
TIME (SEC)

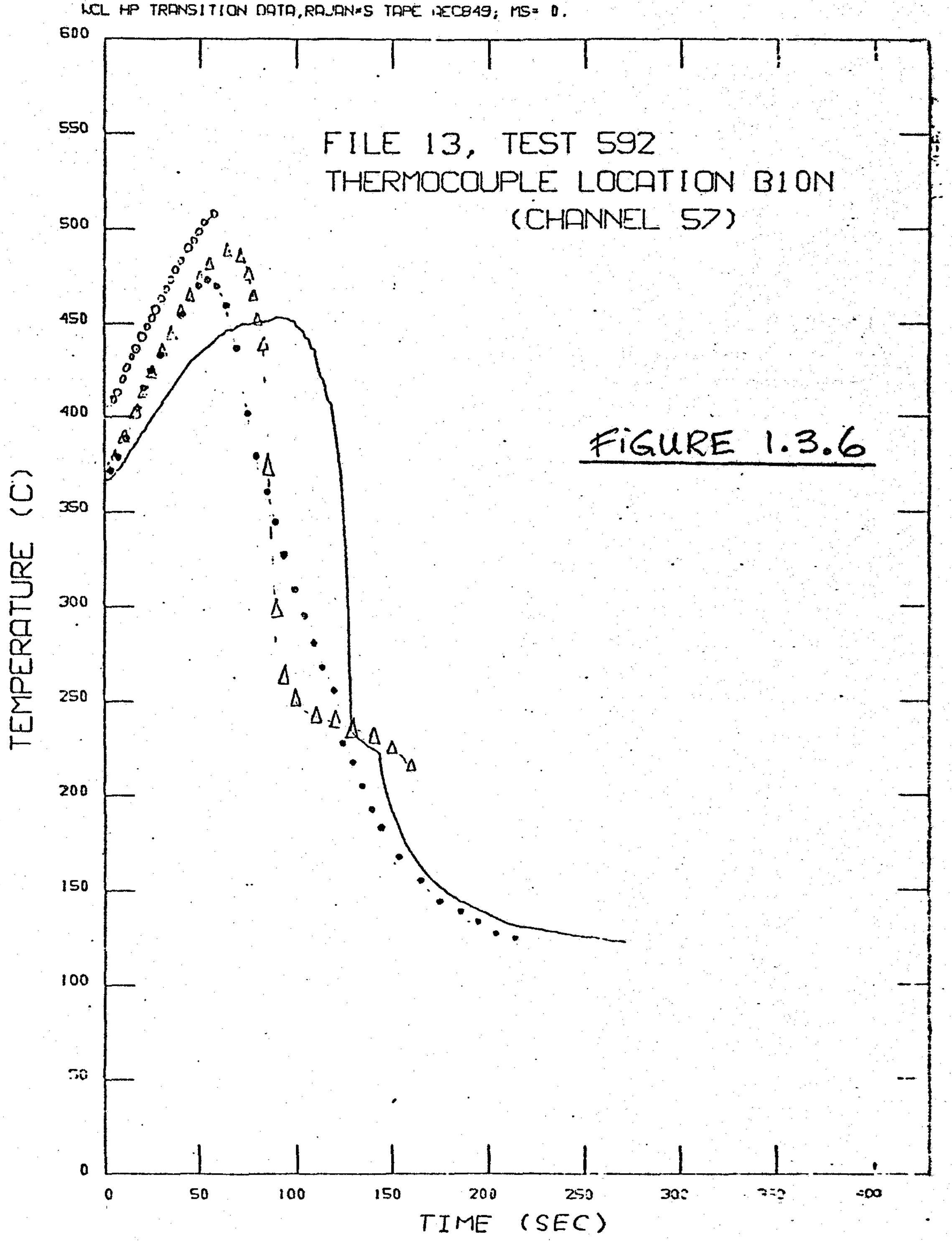

WCL HP TRANSITION DATA, RAJAN*S TAPE REC849; MS= 0.
FILE 13, TEST 592
THERMOCOUPLE LOCATION B10N
(CHANNEL 57)
TEMPERATURE (C)
0
50
100
150
200
250
300
350
400
450
500
550
600
TIME (SEC)
0
50
100
150
200
250
300
350
400

FIGURE 1.3.6

CHAPTER 2

THE WATER PACKING PROBLEM

2.1 Problem Definition

In the porching implicit scheme used in Firebird, the solution variables are:

$M \equiv$ Nodal mass

$U \equiv$ Total internal energy

$W \equiv$ Mass flow rate at the node boundaries

The nodal pressure is advanced in time by the formula

$$p^{n+1} = p^{n} + \Delta p \tag{2.1.1}$$

where Δp is approximated by:

$$\Delta p = \left(\frac{\partial p}{\partial M}\right)_U \Delta M + \left(\frac{\partial p}{\partial U}\right)_M \Delta U \tag{2.1.2}$$

and the partial derivatives above are evaluated at time level $n\Delta t$.

The partial derivatives of equation 2.1.2 are discontinuous at the phase boundaries and severe pressure spikes can result if one attempts to simulate a phase transition using this method.

The discontinuity at a 2 phase-superheated boundary is somewhat mild and poses no problem of practical important. The subcooled-2 phase discontinuity is severe and will be considered here.

The physical reason behind this phenomenum is not difficult to understand. Consider a node L units long which initially contains superheated steam. At time $t = 0$ subcooled water starts to move from the left boundary towards the right with a constant velocity v so that it will reach the right hand boundary at

$$t = t_f = \frac{L}{v} \tag{2.1.3}$$

The homogeneous quality of this node can then be given as a function of time as:

$$x(t) = \begin{cases} \geq 1 & t = 0 \\ 0 < x < 1 & 0 < t < t_f \\ \leq 0 & t \geq t_f \end{cases} \tag{2.1.4}$$

Let's now consider what happens if we try to apply equation 2.1.2 to update the pressure in this particular problem. For $0 < t < t_f$ The pressure at a new time step is given by:

$$p_{2\phi}^{n+1} = p_{2\phi}^{n} + \left(\frac{\partial p}{\partial M}\right)_{2\phi} \Delta M_{2\phi} + \left(\frac{\partial p}{\partial U}\right)_{2\phi} \Delta U_{2\phi} \tag{2.1.5}$$

where the subscript 2ϕ implies that these are in the 2-phase region. For $t \geq t_f$ the new pressure is given by:

$$p_{f}^{n+1} = p_{f}^{n} + \left(\frac{\partial p}{\partial M}\right)_{f} \Delta M_{f} + \left(\frac{\partial p}{\partial U}\right)_{f} \Delta U_{f} \tag{2.1.6}$$

where the subscript f means that these derivatives are in the subcooled region.

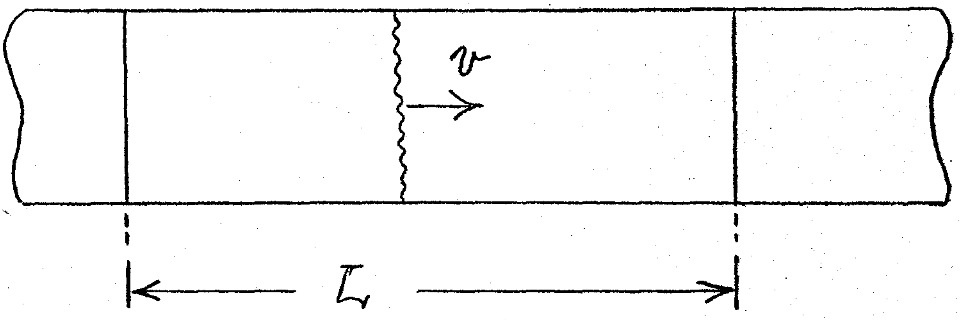


Figure 2.1.1: A transition Node

Subtracting equation 2.1.5 from equation 2.1.6 and using the symbol Δp for the change in pressure over one time step we get:

$$(\Delta p_f - \Delta p_{2\phi}) = [\left(\frac{\partial p}{\partial M}\right)_f \Delta M_f - \left(\frac{\partial p}{\partial M}\right)_{2\phi} \Delta M_{2\phi}]$$

$$+ [\left(\frac{\partial p}{\partial U}\right)_f \Delta U_f - \left(\frac{\partial p}{\partial U}\right)_{2\phi} \Delta U_{2\phi}] \qquad (2.1.7)$$

The left hand side of the above equation is an expression for the change in the change in pressure which is produced when one attempts to use this method of solution for a subcooled-two phase boundary. If this change is large it will cause a pressure spike.

We can work through a simple numerical example to get a feeling for the magnetudes involved. Consider three adjacent nodes as in Figure 2.1.2. The characteristics of the problem are as follows:

Dimensions

$\Delta x_1 = \Delta x_2 = \Delta x_3 = 1m$

$A_1 = A_2 = A_3 = 1m^2$

$V_1 = V_2 = V_3 = 1m^3$

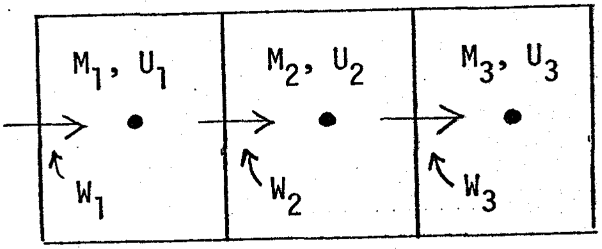


Figure 2.1.2: Threee adjacent nodes in the staggered mesh system.

Initial Condition

$p_1 = p_2 = p_3 = 1$ MPa

$x_1 \equiv$ slightly subcooled

$x_2 = 10^{-3}$

$u_1 = 0$ m/sec

$u_2 = 14.62$ m/sec

$u_3 = 0$ m/sec

Fluid $\equiv$ water

Boundary Conditions

$p_1 \equiv p_3 \equiv$ constant $= 1$ MPa

$W_1 = 0$, M_1 and U_1 Held constant

Time Step

DT = 0.01 secs

At this thermodynamic state the properties are found[1] to be:

$\rho_g = 5.147$ kg/m^3; $\rho_f = 887.0$ kg/m^3

$e_g = 2.582*10^6$ J/kg; $e_f = 7.615*10^5$J/kg

Thus the initial value of the independent variables are:

Mass:

$$M_1^{\circ} \approx V_1\rho_f = 887.0 \text{ kg}$$

$$M_2^{\circ} = \frac{V_2}{xv_g + (1-x)v_f} = 757.3 \text{ kg}$$

Mass Flow Rate:

$$W_1^{\circ} = 0$$

$$W_2^{\circ} = \frac{\overset{\circ}{M}_1\overset{\circ}{u}_2}{\Delta x_1} = 887.0*14.62 = 1.297*10^4 \text{ kg/sec}$$

$$W_3^{\circ} = 0$$

Energy:

$$U_1^{\circ} = M_1^{\circ} e_1^{\circ} \approx M_1^{\circ} e_f = 6.754*10^8 \text{ Joules}$$

$$U_2^{\circ} = M_2^{\circ}[x_2 e_g + (1-x_2)e_f] = 5.750*10^8 \text{ Joules}$$

For simplicity let the time increment of the independent variables be given by the simple explicit scheme:

$$\Delta M_j = \Delta t[W_j^n = W_{j+1}^n]$$

$$\Delta W_j = \Delta t\{(u_{j-1}^n W_{j-1}^n - u_j^n W_j^n) + (p_{j-1}^n - p_j^n)\}$$

$$\Delta U_j = \Delta t\{u_j^n(U_{j-1}^n + p_{j-1}^n) - u_{j+1}^n(U_j^n + p_j^n)\}$$

In the above equations all factors which included Δx, A or V were ignored since they have unit value in this problem.

The solution can now be advanced in time

1st Time Step

Time = DT = 0.01 secs

Mass

$$\Delta M_2 = 0.01\ (1.297*10^4 - 0) = 129.7 \text{ kg}$$

$$\therefore M_2^1 = M_2^{\circ} + \Delta M_2 = 757.3 + 129.7 = 887.0 \text{ kg}$$

Mass Flow Rate

$$\Delta W_2 = 0.01\{(0 - 14.62*1.297*10^4) + 0\} = -1.896*10^3 \ \frac{\text{kg}}{\text{sec}}$$

$$\therefore W_2^1 = W_2^{\circ} + \Delta W_2 = 1.297*10^4 - 1.896*10^3 = 1.107*10^4 \ \frac{\text{kg}}{\text{sec}}$$

$$U_2^1 = \frac{W_2^1}{M_1^1} = \frac{1.107*10^4}{887.0} = 12.48 \text{ m/sec}$$

$$\Delta W_3 = 0.01\ \{(14.62*1.297*10^4-0)+0\} = 1.896*10^3\ \frac{kg}{sec}$$

$$\therefore\ W_3^1 = W_3^{\circ} + \Delta W_3 = 0 + 1.896*10^3 = 1.896*10^3\ kg/sec$$

$$U_3^1 = \frac{W_3^1}{M_2^1} = \frac{1.896*10^3}{887.0} = 2.138\ m/sec$$

Energy

$$\Delta U_2 = 0.01\{14.62(6.754*10^8+10^6) - 0\} = 9.889*10^7\ Joules$$

$$\therefore U_2^1 = U_2^o + \Delta U_2 = (5.750+0.9889)*10^8 = 6.739*10^8\ Joules$$

Quality

$$x_2^1 = \left[\frac{V - Mv_f}{M(v_g - v_f)}\right] \simeq 0 \quad \text{(slightly subcooled)}$$

Pressure

$$\Delta p_2 = \left(\frac{\partial p}{\partial M}\right)_U \Delta M_2 + \left(\frac{\partial p}{\partial U}\right)_M \Delta U_2$$

$$= 5.151*10^3*129.7 + 6.860*10^{-3}*9.889*10^7$$

$$= 1.030*10^4\ \ Pascals$$

The partial derivatives used above are calculated in Appendix 1.

$$\therefore\ p_2^1 = p_2^o + \Delta p_2 = 1.010*10^6\ Pascals$$

Enthalpy

$$h_2^1 = \left(\frac{U_2^1}{M_2^1}\right) + \left(\frac{V\ p_2^1}{M_2^1}\right) = \frac{1}{M_2^1}\ [U_2^1 + V\ p_2^1]$$

$$= \left(\frac{1}{887.0}\right)\ [6.739*10^8 + 1.010*10^6] = 7.609*10^5\ \frac{Joules}{kg}$$

The solution can now be advanced one more time step. Node #2 is already completely filled with water thus its properties will be in the subcooled region.

2nd Time Step

Time = 2.0*DT = 0.02

Mass

$$\Delta M_2 = 0.01\ (1.107*10^4 - 1.896*10^3) = 91.74 \text{ kg}$$

$$\therefore M_2^2 = M_2^1 + \Delta M = 978.7 \text{ kg}$$

Mass Flow Rate

$$\Delta W_2 = 0.01\ \{(0-12.48*1.107*10^4) + (10^6-1.010*10^6)\}$$

$$= 1.482*10^3 \text{ kg/sec}$$

$$W_2^2 = W_2^1 + \Delta W_2 = 1.107*10^4 - 1.482*10^3 = 9.588*10^3\ \frac{\text{kg}}{\text{sec}}$$

$$U_2^2 = \frac{W_2^2}{M_1^2} = \frac{9.588*10^3}{887.0} = 10.81 \text{ m/sec}$$

$$\Delta W_3 = 0.01\ \{(12.48*1.107*10^4-2.138*1.896*10^3) + 0.010*10^6\}$$

$$= 1.441*10^3 \text{ kg/sec}$$

$$W_3^2 = W_3^1 + \Delta W_3 = 1.896*10^3 + 1.441*10^3 = 3.337*10^3\ \frac{\text{kg}}{\text{sec}}$$

$$U_3^2 = \frac{W_3^2}{M_2^2} = \frac{3.337*10^3}{978.7} = 3.410 \text{ m/sec}$$

Energy

$$\Delta U_2 = 0.01\ \{12.48(6.754*10^8+10^6) - 2.138(6.739*10^8+1.01*10^6)\}$$

$$= 6.999*10^7 \text{ Joules}$$

$$U_2^2 = U_2^1 + \Delta U_2 = 6.739*10^8 + 6.999*10^7 = 7.439*10^8 \text{ Joules}$$

We are now in the position to update the pressure once again. However the partial derivatives used are taken from the subcooled region this time, the details of this calculation can be found in Appendix 1.

Pressure

$$\Delta p_2 = \left(\frac{\partial p}{\partial M}\right)_U \Delta M + \left(\frac{\partial p}{\partial M}\right)_M \Delta U$$

$$= 1.126*10^6*91.74 + 3.945*10^{-1}*6.999*10^7$$

$$= 1.309*10^8 \text{ Pascals}$$

$$\therefore p_2^2 = p_2^1 + \Delta p_2 = 1.319*10^8 \text{ Pascals}$$

The effect of this pressure rise on the velocity field can also be calculated:

3rd Time Step

Time = 3.0*DT = 0.03 secs

Mass:

$$\Delta M_2 = 0.01\ (9.588*10^3 - 3.337*10^3) = 62.51 \text{ kg}$$

$$M_2^3 = M_2^2 + \Delta M_2 = 1.041*10^3 \text{ kg}$$

Mass Flow Rate

$$\Delta W_2 = 0.01\ \{(0-10.81*9.588*10^3) + (10^6 - 1.319*10^8)\}$$

$$= -1.310*10^6 \text{ kg/sec}$$

$$W_2^3 = W_2^2 + \Delta W = 9.588*10^3 - 1.310*10^6 = -1.300*10^6 \frac{\text{kg}}{\text{sec}}$$

$$U_2^3 = \frac{W_2^3}{M_2^3} = \frac{-1.300*10^6}{1.041*10^3} = -1.249*10^3 \frac{\text{m}}{\text{sec}}$$

$$\Delta W_3 = 0.01\ \{(10.81*9.588*10^3 - 3.410*3.337*10^3) + (1.319*10^8 - 10^6)\}$$

$$= 1.310*10^8 \text{ kg/sec}$$

$$W_3^3 = W_3^2 + \Delta W = 3.337*10^3 + 1.310*10^8 = 1.310*10^8 \text{ kg/sec}$$

$$U_3^3 = \frac{W_3^3}{M_2^3} = \frac{1.310*10^8}{1.041*10^3} = 1.258*10^3 \text{ m/sec}$$

The change in the change in pressure for the second node of this example can now be calculated from equation 2.1.7:

$$(\Delta p_f - \Delta p_{2\phi}) = 1.309*10^8 - 1.030*10^4 \approx 1.309*10^8 \text{ Pascals}$$

Thus in this case the change in the change in pressure as the node filled up is over one hundred times the nodal pressure itself which in reality is an extremely severe pressure spike, this sudden rise in pressure was so gigantic in fact that it caused a splitting flow of hypersonic proportion.

Clearly this is a completely non-physical phenomenum. From the mathematical point of view it is quite easy to explain why these peculiar solutions are being obtained. The partial derivatives of pressure are highly discontinuous at the phase boundaries, and in fact they are not even defined at these boundaries, this can be easily verified by referring to the usual p-v-T diagram of figure 2.1.3. The lines of constant temperature on the surface of this diagram are not smooth at the phase boundaries, which implies in fact that $(\frac{\partial p}{\partial v})$ does not exist there. And since $(\frac{\partial p}{\partial M})$ is a function of $(\frac{\partial p}{\partial v})$ it can easily be concluded that $(\frac{\partial p}{\partial M})$ does not exist at these boundaries either. The same types of argument can be used for $(\frac{\partial p}{\partial U})$ if one consideres the lines of constant specific volume.

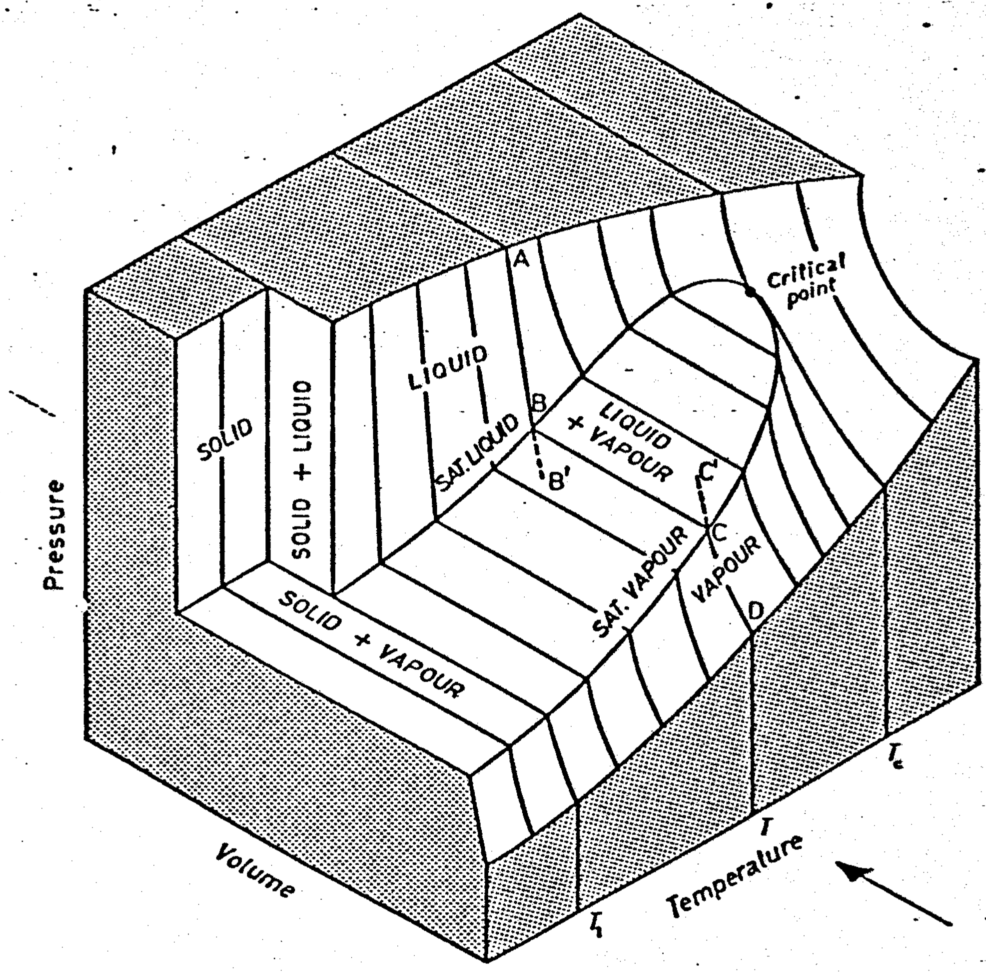


Fig. 2.1.3: Pressure–Volume–Temperature Surface for a Pure Substance

Thus at the phase boundaries the partial derivatives of pressure with respect to the independent variables are not only highly discontinuous but they do not exist there, thus any attempt to simulate a transition node with a set of partial differential equations is clearly inconsistent since by definition differential equations can only represent processes which are continuous and differentiable. Thus in general the results of such a simulation cannot represent the physical behaviour of the process being simulated and it is quite conceivable (as it was shown by the numberical example worked out) that in some cases these results will have no similarity to the real phenomenum whatsoever.

The partial differential equations approach can be used on both sides of the boiling boundary but not across it. The boiling boundary itself cannot be included in the solution domain of these P.D.E. and must be treated separately.

Before we consider a new approach to the problem we must first be able to identify these transition nodes. This will be done in the next section.

2.2 Transition Node Identification

Consider three adjacent nodes as in figure 2.2.1. In accordance with the staggered mesh used in the porsching scheme the thermo static properties are defined at the node centre and the mass flow rate at the node boundaries.

We would like to be able to systematically identify when the jth node becomes a transition node just by knowing the thermonamic properties at all three nodes.

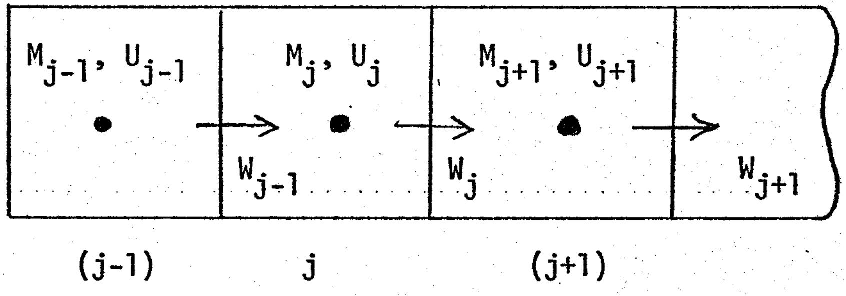


Figure 2.2.1: Three adjacent nodes in the staggered mesh system.

Let Y be a number which contains five binary digits.

$$Y = A_1\ A_2\ A_3\ A_4\ A_5$$

where:

$$\left.\begin{array}{l} A_1 \equiv \text{phase of } (j-1)^{th} \text{ node} \\ A_2 \equiv \text{phase of } j^{th} \text{ node} \\ A_3 \equiv \text{phase of } (j+1)^{th} \text{ node} \end{array}\right\} = \left\{\begin{array}{l} 0 \text{ if } x<0 \\ \\ 1 \text{ if } x \geq 0 \end{array}\right.$$

$$\left.\begin{array}{l} A_4 \equiv \text{flow direction of } (j-1)^{th} \text{ node} \\ A_5 \equiv \text{flow direction of } j^{th} \text{ node} \end{array}\right\} = \left\{\begin{array}{l} 0 \text{ if -ve} \\ 1 \text{ if +ve} \end{array}\right.$$

Thus for example the configuration of figure 2.2.2 has associated with it a value of Y of:

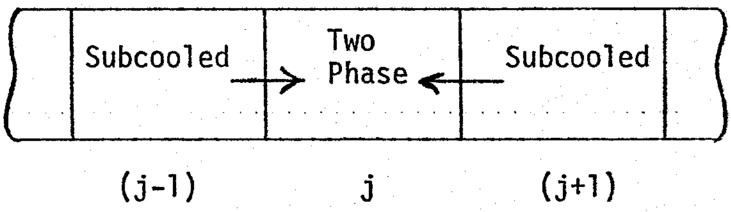
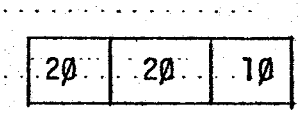
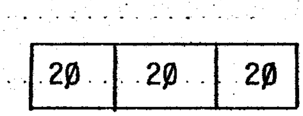


Figure 2.2.2: A particular combination of flow directions and thermodynamic phases.

Y - 01010 = 10_{Decimal}

The total number of possible combinations amounts to thrity two. Let the symbols 1Ø and 2Ø represent subcooled and two-phase properties respectively. A pictorial representation of all the possible combinations can be drawn:

Decimal Equivalent	A_1	A_2	A_3	A_4	A_5	Symbolic phasic diagram
0	0	0	0	0	0	1Ø 1Ø 1Ø
1	0	0	0	0	1	
2	0	0	0	1	0	
3	0	0	0	1	1	
4	0	0	1	0	0	1Ø 1Ø 2Ø
5	0	0	1	0	1	
6	0	0	1	1	0	
7	0	0	1	1	1	
8	0	1	0	0	0	1Ø 2Ø 1Ø
9	0	1	0	0	1	
10	0	1	0	1	0	
11	0	1	0	1	1	
12	0	1	1	0	0	1Ø 2Ø 2Ø
13	0	1	1	0	1	
14	0	1	1	1	0	
15	0	1	1	1	1	
16	1	0	0	0	0	2Ø 1Ø 1Ø
17	1	0	0	0	1	
18	1	0	0	1	0	
19	1	0	0	1	1	
20	1	0	1	0	0	2Ø 1Ø 2Ø
21	1	0	1	0	1	
22	1	0	1	1	0	
23	1	0	1	1	1	

Decimal Equivalent	A_1	A_2	A_3	A_4	A_5	Symbolic phasic diagram
24	1	1	0	0	0	
25	1	1	0	0	1	
26	1	1	0	1	0	
27	1	1	0	1	1	
28	1	1	1	0	0	
29	1	1	1	0	1	
30	1	1	1	1	0	
31	1	1	1	1	1	

By referring to the symbolic phasic diagrams for the different combinations it can be seen that in one time step the following combinations (their decimal equivalent) will never make the jth node go through the subcooled two phase transition:

Combination: 0, 1, 2, 3, 4, 5, 6, 7, 8, 16, 17, 18, 19, 28, 29, 30, 31

In fact the only ones that may pose a problem are:

Combinations: 8, 10, 11, 14, 15, 24, 26

The other combinations can never make the jth node go through a subcooled two phase transition over the span of one time step.

It is thus possible to identify when a node may go through a transition so that some precautionary measures may be taken.

This method of identification has been implemented in one version of Firebird and is fully operational now. See Appendix 3 for the listing.

2.3 The Method of Power Series Expansion

As it was shown in Section 2.1 of this report the "water-packing" problem occurs because one tries to use a set of differential equations to represent the discontinuous processes which occur across a boiling boundary. However on each side of this boundary all the thermodynamic properties are differentiable and continuous and have continuous first derivatives, thus they can rightfully be represented by the differential equations approach.

In this section a procedure for dealing with the boiling boundary is proposed. This procedure can accurately locate the boundary position and gives an approximate value of the thermodynamic proeprties on each side by the method of power series expansion. It is assumed here that the properties at the boundary are in the saturated state.

Consider a boiling boundary which is going through a node bounded by the co-ordinates z_j and z_{j+1} as in figure 2.3.1. Let the position of the boiling boundary be denoted by z_f where:

$$z_j < z_f < z_{j+1}$$

At the boiling boundary the density and internal energy per unit volume are given by

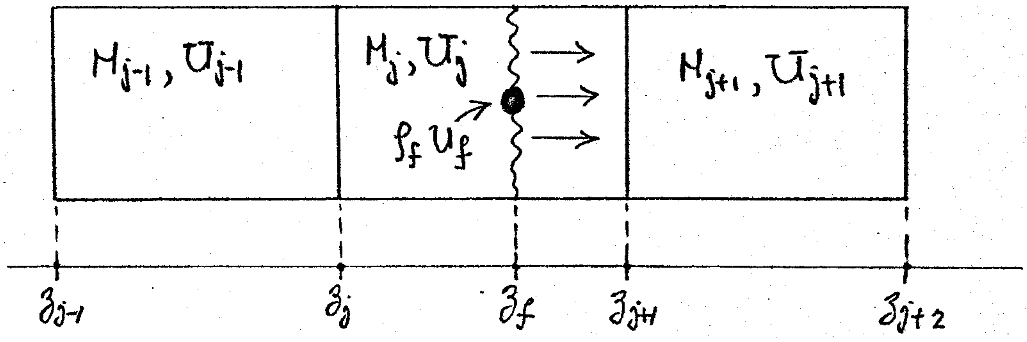


Figure 2.3.1: The boiling boundary.

$$\rho = \rho_f$$

$$u = \rho e = \rho_f e_f = u_f$$

The vlaue of these properties at other places in the node can be approximated by a first order Taylor series expansion.

$$\rho(z) = \begin{cases} \rho_f + (z-z_f) \left(\frac{\partial\rho}{\partial z}\right)_f & \text{for } z<z_f \\ \rho_f + (z-z_f) \left(\frac{\partial\rho}{\partial z}\right)_{j+1} & \text{for } z>z_f \end{cases} \qquad (2.3.1)$$

$$u(z) = \begin{cases} u_f + (z-z_f) \left(\frac{\partial u}{\partial z}\right)_f & \text{for } z<z_f \\ u_f + (z-z_f) \left(\frac{\partial u}{\partial z}\right)_{j+1} & \text{for } z\geq z_f \end{cases} \qquad (2.3.2)$$

For simplicity let the nodal volume be $V_j = A_j(z_{j+1}-z_j)$

$$\therefore M_j = A_j \int_{z_j}^{z_{j+1}} \rho(z)dz \qquad (2.3.3)$$

$$U_j = A_j \int_{z_j}^{z_{j+1}} u(z)dz \qquad (2.3.4)$$

Substituting for $\rho(z)$ from equation 2.3.1 into equation 2.3.3:

→

$$M_j = A\{ \int_{z_j}^{z_f} [\rho_f + (z-z_f) \left(\frac{\partial\rho}{\partial z}\right)_f]dz$$

$$+ \int_{z_f}^{z_{j+1}} [\rho_f + (z-z_f) \left(\frac{\partial\rho}{\partial z}\right)_{j+1}]dz\}$$

$$= A\{\rho_f(z_{j+1}-z_j) + \left(\frac{\partial\rho}{\partial z}\right)_f [\frac{z^2}{2} - zz_f]_{z_j}^{z_f}$$

$$+ \left(\frac{\partial\rho}{\partial z}\right)_{j+1} \left[\frac{z^2}{2} - zz_f\right]_{z_f}^{z_{j+1}} \}$$

$$M_j = A_j\{\rho_f(z_{j+1}-z_j) + \left(\frac{\partial\rho}{\partial z}\right)_f [z_f(z_j-0.5z_f) - 0.5\ z_j^2]$$

$$+ \left(\frac{\partial\rho}{\partial z}\right)_{z+1} [z_{j+1}(0.5z_{j+1}-z_f) + 0.5\ z_f^2]\} \qquad (2.3.5)$$

Following the same procedure we get a similar expression for U_j

→

$$U_j = A_j\{U_f(z_{j+1}-z_j) + \left(\frac{\partial u}{\partial z}\right)_f [z_f(z_j-0.5z_f) - 0.5z_j^2]$$

$$+ \left(\frac{\partial u}{\partial z}\right)_{j+1} [z_f(0.5z_f-z_{j+1}) + 0.5z_{j+1}^2]\} \qquad (2.3.6)$$

The properties at the adjacent node can also be approximated by:

$$M_{j+1} = A_{j+1}\{ \int_{z_{j+1}}^{z_{j+2}} [\rho_f + (z-z_f)\left(\frac{\partial\rho}{\partial z}\right)_{j+1}]dz\}$$

$$= A_{j+1}\{\rho_f(z_{j+2}-z_{j+1}) + \left(\frac{\partial\rho}{\partial z}\right)_{j+1} [0.5z^2 - zz_f]_{z_{j+1}}^{z_{j+2}}\}$$

$$M_{j+1} = A_{j+1}\{\rho_f(z_{j+2}-z_{j+1}) + \left(\frac{\partial\rho}{\partial z}\right)_{j+1} [z_{j+2}(0.5z_{j+2} - z_f)$$

$$-z_{j+1}(0.5z_{j+1}-z_f)]\} \qquad (2.3.7)$$

and similarly:

$$U_{j+1} = A_{j+1}\{U_f(z_{j+2}-z_{j+1}) + \left(\frac{\partial u}{\partial z}\right)_{j+1} [z_{j+2}(0.5z_{j+2} - z_f)$$

$$-z_{j+1}(0.5z_{j+1}-z_f)]\} \qquad (2.3.8)$$

The value of the partial derivatives at the position z_{j+1} can thus be obtained from equations 2.3.7 and 2.3.8.

$$\left(\frac{\partial\rho}{\partial z}\right)_{j+1} = \frac{M_{j+1} - A_{j+1}[\rho_f(z_{j+2}-z_{j+1})]}{A_{j+1}[z_{j+2}(0.5z_{j+2}-z_f) - z_{j+1}(0.5z_{j+1}-z_f)]} \qquad (2.3.9)$$

$$\left(\frac{\partial u}{\partial z}\right)_{j+1} = \frac{U_{j+1} - A_{j+1}[U_f(z_{j+2}-z_{j+1})]}{A_{j+1}[z_{j+2}(0.5z_{j+2}-z_f) - z_{j+1}(0.5z_{j+1}-z_f)]} \qquad (2.3.10)$$

The values above can now be substituted into equations 2.3.5 and 2.3.6:

→

$$\left(\frac{\partial\rho}{\partial z}\right)_{f} = \frac{M_j-A_j\rho_f(z_{j+1}-z_j)]*[z_{j+2}(0.5z_{j+2}-z_f)-z_{j+1}(0.5z_{j+1}-z_f)}{\text{DENOM}}$$

$$- \frac{(M_{j+1}-A_{j+1}\rho_f(z_{j+2}-z_{j+1})]*[z_{j+1}(0.5z_{j+1}-z_f) + 0.5z_f^2]}{\text{DENOM}} \qquad (2.3.11)$$

$$\left(\frac{\partial u}{\partial z}\right)_{f} = \frac{[U_j-A_jU_f(z_{j+1}-Z_j)]*[z_{j+2}(0.5z_{j+2}-z_j)-z_{j+1}(0.5z_{j+1}-z_f)]}{\text{DENOM}}$$

$$- \frac{[U_{j+1}-A_{j+1}U_f(z_{j+1}-z_{j+1})]*[z_{j+1}(0.5z_{j+1}-z_f) + 0.5z_f^2}{\text{DENOM}} \qquad (2.3.12)$$

where:

$$\text{DENOM} = \{A_{j+1}[z_f(z_j-0.5z_f)-0.5z_f) - 0.5z_j^2]*[z_{j+2}(0.5z_{j+2}-z_f)$$
$$-z_{j+1}(0.5z_{j+1}-z_f)]$$

The partial derivatives given by equations 2.3.11 and 2.3.12 are fully determined except for z_f which is not known. However its value can be calculated by the following method: let's assume that $\frac{dp}{dz}$ is constant across the boundary

$$\therefore \left(\frac{dp}{dz}\right)_f = \left(\frac{dp}{dz}\right)_{j+1}$$

$$\rightarrow \left(\frac{\partial p}{\partial \rho}\right)_f \left(\frac{\partial \rho}{\partial z}\right)_f + \left(\frac{\partial p}{\partial u}\right)_f \left(\frac{\partial u}{\partial z}\right)_f = \left(\frac{\partial p}{\partial \rho}\right)_{j+1} \left(\frac{\partial p}{\partial z}\right)_{j+} + \left(\frac{\partial p}{\partial u}\right)_{j+1} \left(\frac{\partial u}{\partial z}\right)_{j+1} \qquad (2.3.13)$$

The partial derivatives of pressure with respect to δ and u can be found by knowing the local thermodynamic state which is the case here. If we substitute for

$$\left(\frac{\partial \rho}{\partial z}\right)_{j+1}; \left(\frac{\partial u}{\partial z}\right)_{j+1}; \left(\frac{\partial \rho}{\partial z}\right)_f \text{ and } \left(\frac{\partial u}{\partial z}\right)_f$$

from equations 2.3.9 to 2.3.12 respectively into equation 2.3.13 we then have an equation in which the only unknown is z_f and it can be solved for.

One the value of z_f is known then the partial derivatives of δ and u w.r.t. the distance z at the boiling boundary are completely determined by the expressions given by equation 2.3.11 and 2.3.12 respectively.

The thermodynamic properties on both sides of the boiling boundary can now be fully established. The node which contains this boundary can now be divided into two smaller ones such that the first one on the left exactly contains all the water. By following this process at all time steps the boiling boundary will always coincide with a node boundary, and since the pressure is not defined at these boundaries the discontinuities there will not cause any problem. This procedure merely isolates these discontinuities thus making sure that these partial differential equations are truly defined in their entire domain.

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2. Agee, L.J. (1977), "An Analytical Method of Integrating the Thermal-Hydraulic Conservation Equations", Nuclear Engineering and Design, Vol. 42, pp. 195-208.

APPENDIX 1

A1.1 The Partial Derivatives of Water in the Two-Phase Region

By definition

$$v = xv_g + (1-x)v_f \qquad \text{(A1.1.1)}$$

$$h = xhg + (1-x)h_f$$

$$\therefore dv = xdv_g + v_g d_x + dv_f(1-x) - v_f dx$$

$$dh = xdh_g + h_g dx + dh_f(1-x) - h_f dx$$

$$\rightarrow \qquad dx = \frac{dv - xdv_g - (1-x)dv_f}{(v_g - v_f)} = \frac{dh - xdh_g - (1-x)dh_f}{(h_g - h_f)}$$

Multiplying both sides of the above equation by $(v_g-v_f)*(h_g-h_f)$:

$$\rightarrow \qquad (v_g - v_f)[dh - xdh_g - (1-x)dh_f]$$

$$= (h_g - h_f)[dv - xdv_g - (1-x)dv_f] \qquad \text{(A1.1.2)}$$

The specific enthalpy h can be expressed as:

$$h = u + pv = \frac{U}{M} + \frac{pV}{M} \qquad \text{(A1.1.3)}$$

where V is the nodal volume

$$\therefore dh = \frac{1}{M}[dU = \frac{U}{M} dM + V\,dp - \frac{pV}{M} dM]$$

$$= \frac{1}{M}[-(\frac{U}{M} + \frac{pV}{M})dM + dU + Vdp]$$

$$\rightarrow \qquad dh = \frac{1}{M}[-hdM + dU + Vdp] \qquad \text{(A1.1.4)}$$

Also the specific volume is given by:

$$v = \frac{V}{M} \therefore dV = \frac{-V}{M^2} dM \qquad \text{(A1.1.5)}$$

Substituting for dh and dv from above into equation A1.1.2:

$$\rightarrow \qquad (v_g-v_f)\{\tfrac{1}{M}[-hdM+dU+Vdp]-xdhg - (1-x)dh_f\}$$

$$=(h_g-h_f)\{\frac{-V}{M^2}\,dM - xdV_g - (1-x)dV_f\} \qquad \text{(A1.1.6)}$$

The differentials of specific enthalpy and specific volumes at saturation which appear in the equation above can be expressed as:

$$\begin{aligned} dh_s &= \left(\frac{dh_s}{dp}\right) dp \\ dV_s &= \left(\frac{dV_s}{dp}\right) dp \end{aligned} \qquad \text{(A1.1.7)}$$

Thus equation A1.1.6 can be rewritten as:

$$(v_g-v_f)\{dM[\frac{-h}{M}] + dU[\frac{1}{M}] + dp[\frac{V}{M} - x(\frac{dh_g}{dp}) - (1-x)(\frac{dh_f}{dp})]\}$$

$$= (h_g-h_f)\{dM[\frac{-V}{M^2}] + dp[-x(\frac{dV_g}{dp}) - (1-x)(\frac{dv_f}{dp})]\}$$

Multiplying through by M

$$\rightarrow \qquad dp\{(v_g-v_f)[V - Mx(\frac{dh_g}{dp}) - M(1-x)(\frac{dh_f}{dp})]$$

$$+(h_g-h_f)[Mx(\frac{dv_g}{dp}) + M(1-x)(\frac{dv_f}{dp})]\}$$

$$=dM[h(v_g-v_f) - v(h_g-h_f)] - dU[(v_g-v_f)]$$

Thus

$$\left(\frac{\partial p}{\partial M}\right)_U = \frac{h(v_g-v_f) - v(h_g-h_f)}{\text{DENOM}} \qquad \text{(A1.1.8)}$$

$$\left(\frac{\partial p}{\partial U}\right)_M = \frac{-(v_g-v_f)}{\text{DENOM}} \qquad \text{(a1.1.9)}$$

where:

$$\text{DENOM} = M\{(h_g-h_f)[x(\frac{dv_g}{dp}) + (1-x)(\frac{dv_f}{dp})]$$

$$-(v_g-v_f)[x(\frac{dh_g}{dp}) + (1-x)(\frac{dh_f}{dp}) - v]\}$$

At $p = 1$ Mpa and $x = 10^{-3}$ the value of the thermodynamic properties for saturated steam and water mixture are given by [1]:

$$v_f = 1.127*10^{-3}\ \frac{m^3}{kg};\ v_g = 1.943*10^{-1}\ \frac{m^3}{kg}$$

$$h_f = 7.626*10^5\ \frac{\text{Joules}}{kg};\ h_g = 2.776*10^6\ \frac{\text{Joules}}{kg}$$

$$\left(\frac{dh_f}{dp}\right) = 1.922*10^{-1}\ \frac{m^3}{kg};\ (\frac{dh_g}{dp}) = 3.859*10^{-2}\ \frac{m^3}{kg}$$

$$\left(\frac{dv_f}{dp}\right) = 5.903*10^{-11}\ \frac{m^5}{(N\text{-}kg)};\ \left(\frac{dv_g}{dp}\right) = -1.852*10^{-7}\ \frac{m^5}{(N\text{-}kg)}$$

$$v = xv_g + (1-x)v_f$$

$$= 10^{-3}*1.943*10^{-1} + 0.999*1.127*10^{-3} = 1.320*10^{-3}\ \frac{m^3}{kg}$$

$$h = xh_g + (1-x)h_f$$

$$= 10^{-3}*2.776*10^6 + 0.999*7.626*10^5 = 7.646*10^5$$

$$\therefore \text{DENOM} = 757.3\{(2.776-0.7626)*10^6*[-1.852*10^{-10}$$

$$+0.999*5.903*10^{-11}] - (1.943 - 0.01127)*10^{-1}*[3.859*10^{-5}$$

$$+0.999*1.922*10^{-1} - 1.320*10^{-3}]\}$$

$$= 757.3\{-3.425*10^{-4} - 3.684*10^{-2}\}$$

→ $\text{DENOM} = -28.16$

$$\therefore \left(\frac{\partial p}{\partial M}\right)_U = \frac{h(v_g-v_f)-v(h_g-h_f)}{\text{DENOM}}$$

$$= \left(\frac{-1}{28.16}\right)*\{7.646*10^5(1.943*10^{-1}-1.127*10^{-3})$$

$$- 1.320*10^{-3}(2.776*10^6-7.626*10^5)\}$$

$$\rightarrow \qquad \left(\frac{\partial p}{\partial M}\right)_U = -5.151*10^3 \frac{\text{Pascal}}{\text{kg}}$$

$$\left(\frac{\partial p}{\partial U}\right)_M = \frac{-(v_g-v_f)}{\text{DENOM}}$$

$$= \frac{(1.943*10^{-1}-1.127*10^{-3})}{28.16} = 6.860*10^{-3} \frac{\text{Pascal}}{\text{Joule}}$$

A1.2 The Partial Derivatives of Subcooled Water

The specific volume of subcooled water at any given state (p,h) can be evaluated by Agee's polynomials[2]

$$v_{sib} = v(p,h) \qquad \text{(A1.2.1)}$$

$$\therefore dv = \left(\frac{\partial v}{\partial p}\right)dp + \left(\frac{\partial v}{\partial h}\right)dh \qquad \text{(A1.2.2)}$$

The specific enthalpy in british units can be expressed as:

$$h = u + \frac{pv}{5.4} = \frac{U}{M} + \frac{pV}{5.4M}$$

$$\rightarrow \qquad h = \left(\frac{1}{M}\right)[U + \frac{pV}{5.4}]$$

$$\therefore dh = \left(\frac{1}{M}\right)\{[dU + \frac{V}{5.4}\,dp] - \left(\frac{1}{M}\right)[U + \frac{pV}{5.4}]\,dM\}$$

$$\rightarrow \qquad dh = \frac{1}{M}\,\{[dU + \frac{V}{5.4}\,dp] - h\,dM\}$$

Also

$$v = \frac{V}{M} \quad \therefore dv = \left(\frac{-V}{M^2}\right)dM$$

Substituting for dh and dv into equation A1.2.2 we get:

$$\left(\frac{V}{M^2}\right) dM = -\left(\frac{\partial v}{\partial p}\right) dp + \left(\frac{1}{M}\right)\left(\frac{\partial v}{\partial h}\right)[hdM - (dU + \frac{V}{5.4}dp)]$$

Multiplying the above equation by M and rearranging:

$$dp[M\left(\frac{\partial v}{\partial p} + \frac{v}{5.4}\,\frac{\partial v}{\partial h}\right)]$$

$$= dM[h\frac{\partial v}{\partial h} - v] - dU[\frac{\partial v}{\partial h}]$$

$$\therefore \left.\frac{\partial p}{\partial M}\right)_U = \frac{h\left(\frac{\partial v}{\partial h}\right) - v}{DENOM} \qquad (A1.2.3)$$

$$\left.\frac{\partial p}{\partial U}\right)_M = \frac{-\left(\frac{\partial v}{\partial h}\right)}{DENOM} \qquad (A1.2.4)$$

where $DENOM = M[\left(\frac{\partial v}{\partial p}\right) + \frac{v}{5.4}\left(\frac{\partial v}{\partial h}\right)]$

A simple computer program was written to calculate the partial derivatives given by equations A1.2.3 and A1.2.4. A listing of this program as well as the result output are attached at the end of this appendix. The value of these derivatives are found to be:

$$\left(\frac{\partial p}{\partial M}\right)_U \simeq 1.126*10^6 \frac{\text{Pascal}}{\text{kg}} \qquad (A1.2.5)$$

$$\left(\frac{\partial p}{\partial U}\right)_M \simeq 3.945*10^{-1} \frac{\text{Pascal}}{\text{Joule}} \qquad (A1.2.6)$$

```
      PROGRAM TST (INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION C(5,3)
      DATA(    C(I,1),I=1,5   )/-0.41345E1,0.13252E-4,0.15812E-5,
     1-0.21959E-8,0.21683E-11/
      DATA(    C(I,2),I=1,5   )/-0.59428E-5,0.63377E-7,-0.39974E-9,
     10.69391E-12,-0.36159E-15/
      DATA(    C(I,3),I=1,5   )/0.15681E-8,-0.40711E-10,0.25401E-12,
     1-0.52372E-15,0.32503E-18/
C         THE VALUES OF SPECIFIC ENTHALPY , PRESSURE AND NODAL VOLUME
      RH=7.609E+5
      RP=1.0103E+6
      V=1.0
C         CONVERSION TO BRITISH UNITS
      RP=RP*14.696/1.01325E+5
      RH=RH/(1054.35*2.2046)
      V=V*35.3147
C         THE CALCULATION OF THE DERIVATIVES BY AGEE≠S POLYNOMIALS
      Z=DZDP=DZDH=0.
      DO 10  N=1,3
      DO 10  K=1,5
      Z=Z+C(K,N)*(    RP   **(N-1))*(    RH   **(K-1))
      DZDP=DZDP+FLOAT(N-1)*C(K,N)*(    RP   **(N-2))*(    RH   **(K-1))
      DZDH=DZDH+FLOAT(K-1)*C(K,N)*(    RP   **(N-1))*(    RH   **(K-2))
10    CONTINUE
      VF=EXP(Z)
      DVFDP=DZDP*VF
      DVFDH=DZDH*VF
      DENOM=V*(DVFDP+VF*DVFDH/5.4)/VF
      DPDM=(RH*DVFDH-VF)/DENOM
      DPDU=-DVFDH/DENOM
C         CONVERSION BACK TO METRIC UNITS
      DPDM=DPDM*1.01325E+5*2.2046/14.696
      DPDU=DPDU*1.01325E+5/(14.696*1054.35)
      RP=RP*1.01325E+5/14.696
      RH=RH*1054.35*2.2046
C         WRITE THE RESULTS
      WRITE(6,30) RP,RH,DPDM,DPDU
30    FORMAT(1H1,15(/),10X,≠T H E    P A R T I A L   D E R I V A T I V
     2E S    O F    S U B C O O L E D    W A T E R≠,15(/)
     3,10X,≠P R E S S U R E  =   ≠,E15.8,15X,≠E N T H A L P Y  =  ≠E15.8,
     410(/),15X,≠D P D M  =  ≠,E15.8,20X,≠D P D U  =  ≠,E15.8)
```

```
THE PARTIAL DERIVATIVES OF SUBCOOLED WATER


PRESSURE =   .10103000E+07          ENTHALPY =   .76090000E+06


   DPDM =   .11259188E+07            DPDU =   .39452147E+00
```

APPENDIX 2

```
.*D MAIN.262
.C
.C          GET QUALITY OF ALL NODES
.C
.       DUMMY=PRHG(I)-PRHF(I)
.       IF(DUMMY.EQ.0.) GOTO 169
.       XXX(I)=(HENT(I)-PRHF(I))/DUMMY
.C
.C
.169    CONTINUE
.C
+
.       RUL(I)=0.
.       RUR(I)=VOL(I)
.*I MAIN.262
.       ZSEC=0.1
.       IF(TIME.GT.5.0) ZSEC=0.0
.       IF(TIME.GT.5.5) ZSEC=0.1
.       DO 155 I=1,NE
.C
.C          THE NEXT FEW LINES LOCATES THE BOILING BOUNDARY AND
.C
.C          EVALUATES RIGHT AND LEFT NODAL VOLUMES ...
+
.C
.       M1=I-1
.       M2=I+1
.       IF(I.EQ.1) M1=1
.       IF(I.EQ.NE) M2=NE
.       DUMMY2=XXX(M1)
.       IF(I.EQ.1) DUMMY2=-0.35
.       DUMMY= DUMMY2 -XXX( M2)
.       IF(DUMMY.EQ.0.) GOTO 158
.       IF(XXX(I).GE.1.0) GOTO 158
.       RUL(I)=( DUMMY2 / DUMMY ) * VOL(I)
+
.       IF(RUL(I).LT.0.) RUL(I)=0.
.       IF(RUL(I).GT.VOL(I)) RUL(I)=VOL(I)
.       DUMMY3=DUMMY2*XXX(M2)
.       IF(DUMMY3.GE.0.) RUL(I)=0.
.       IF(IPINJ.EQ.1) GOTO 151
.       IF(PINJ.LE.PRESS(1)) RUL(I)=0.
.       IF(PINJ.LE.PRESS(1)) GOTO 151
.       IPINJ=1
.151    CONTINUE
.       IF(XXX(I).LT.0.) RUL(I)=VOL(I)
.       RUR(I)=VOL(I)-RUL(I)
+
```

```
.158   CONTINUE
.C
.C
.C
.C
.C        RX IS A BINARY DIGIT WHICH TAKES THE VALUE OF ONE IF QUALITY IN THE
.C
.C        NODE IS GREATER THAN ZERO , OTHERWISE IT TAKES THE VALUE OF ZERO
.C
.C
.C
+
.C
.C        RV IS EQUAL TO ONE IF FLOW IN THE NODE IS POSITIVE
.C
.C        OTHERWISE IT IS EQUAL TO ZERO
.C
.C
.      RX(I)=0.
.      RV(I)=0.
.      IF(XXX(I).GT.0.) RX(I)=1.
.      IF(FLOW(I).GT.0.) RV(I)=1.
.155   CONTINUE
+
.      CALL BOILING(NE)
```

```
 .      SUBROUTINE BOILING(NE)
 .      COMMON/STABK/SUEV(70),SVOL(70),DPRESM(70),DPRESU(70)
 .      COMMON/SOIL/RX(70),RV(70),RVL(70),RVR(70),XXX(70)
 .C
 .C
 .C
 .C         THIS SUBROUTINE HANDLES BOILING BOUNDARY DISCONTINUITIES
 .C
 .C         BY EXPRESSING THE DERIVATIVES IN THE TRANSITION NODE AS A
 .C
 .C         COMBINATION OF THE DERIVATIVES OF THE INCOMING FLUID ...
 +
 .C
 .C
 .C
 .C
 .C
 .      DO  300 I=1,NE
 .      VOL=RVL(I)+RVR(I)
 .      M1=I-1
 .      IF(I.EQ.1) M1=1
 .      M2=I+1
 .      IF(I.EQ.NE) M2=NE
 +
 .C
 .C
 .C         D IS THE DECIMAL EQUIVALENT OF  A  BINARY NUMBER DEFINED ACCORDING
 .C
 .C         TO A PRE-SET CONVENTION .... ITS RANGE FROM 0 TO 31 REPRESENTS
 .C
 .C         ALL POSSIBLE COMBINATIONS OF PHASE STATE & FLOW DIRECTIONS ...
 .C
 .C
 .      DUMMY1=RX(M1)
 .      IF(I.EQ.1) DUMMY1=0.
 +
 .      DUMMY2=RV(M1)
 .      IF(I.EQ.1) DUMMY2=1.
 .      D  =  16.0*DUMMY1+8.0*RX(I)+4.0*RX(M2)+2.0*DUMMY2+RV(I)
 .C
 .C
 .C
 .      IF(D.NE.8.AND.D.NE.12.AND.D.NE.24.AND.D.NE.26) GOTO 100
 .      DPRESM(I)=(RVL(I)*DPRESM(I)+RVR(I)*DPRESM(M2))/VOL
 .      DPRESU(I)=(RVL(I)*DPRESU(I)+RVR(I)*DPRESU(M2))/VOL
 .      GOTO 300
 .100   CONTINUE
 +
```