NASA TECHNICAL MEMORANDUM

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AN ANALYTICAL APPROACH TO THERMAL MODELING OF BRIDGMAN-TYPE CRYSTAL GROWTH: ONE-DIMENSIONAL ANALYSIS

Computer Program Users Manual

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May 1982

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George C. Marshall Space Flight Center
Marshall Space Flight Center, Alabama

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16. ABSTRACT

This work documents the computer program written in support of R. J. Naumann's "An Analytical Approach to Thermal Modeling of Bridgman-Type Crystal Growth: One-Dimensional Analysis" (accepted for publication in The Journal of Crystal Growth 1982).

The program listing and flow charts are included, along with the complete thermal model. Sample problems include detailed comments on input and output to aid the first-time user.

This report will be of particular value to the scientific community desiring a one-dimensional analysis of crystal growth to guide more complicated numerical analysis.

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TECHNICAL MEMORANDUM

AN ANALYTICAL APPROACH TO THERMAL MODELING OF BRIDGMAN-TYPE CRYSTAL GROWTH: ONE-DIMENSIONAL ANALYSIS

Computer Program Users Manual

INTRODUCTION

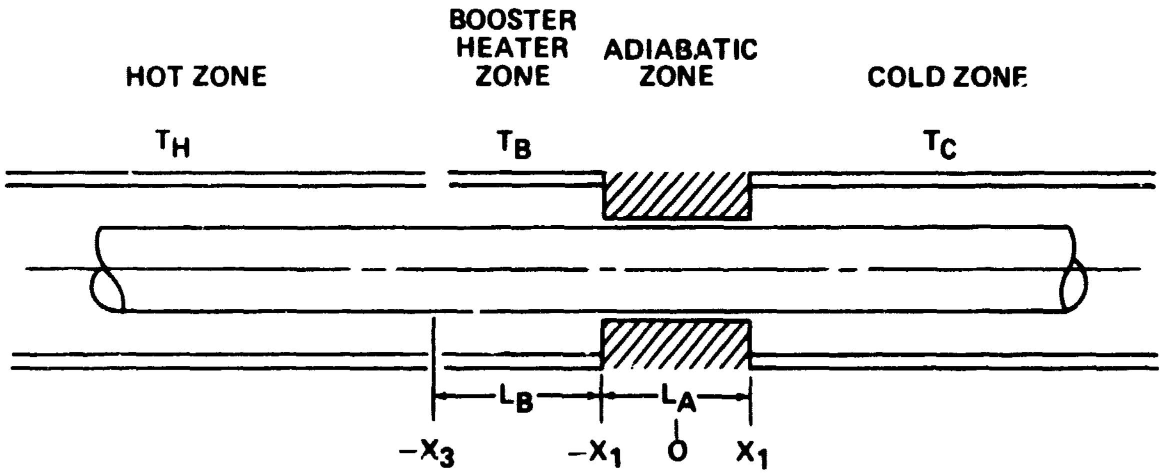
This report is a users guide for a computer program developed to simulate one-dimensional heat flow in a rod inserted into a Bridgeman-type directional solidification furnace. The thermal model was developed by R. J. Naumann of NASA's Space Sciences Laboratory at Marshall Space Flight Center and is included in Appendix B. Using this model, a small scientific computer has been applied to the study of several situations of interest in the Bridgman-type crystal growth. The computer program listing is in Appendix A.

THERMAL MODEL

The complete thermal model for the one-dimensional Bridgman-type crystal growth is included in Appendix B. A brief description follows, but the complete report should be referenced for applications and limitations before attempting to utilize the computer program.

A) The model is a one-dimensional analytical description of heat flow in a translating or motionless rod (sample) inside a directional solidification furnace with an adiabatic zone separating the hot and cold zone.

B) An optional booster (tickler) heater is included in the hot zone just in front of the adiabatic zone.



C) The model is applicable to systems whose Biot numbers in the hot and cold zones are less than unity. The Biot number for the adiabatic zone is assumed equal to zero.

D) Different thermophysical properties of the sample in the solid and liquid state can be accommodated.

E) The space between the sample and furnace wall can be either vacuum or filled with a stagnant or moving fluid. Different heat transfer coefficients in the hot and cold zone can be accommodated.

F) The enclosure of the sample in an ampoule is handled by calculating effective conductivities, specific heat, and density as area weighted averages. These in turn are used to calculate effective Peclet numbers, heat transfer coefficients, and Biot numbers.

$$Kl\ (eff) = Kls \left(\frac{Ain}{Ao}\right)^2 + Ka \left[1 - \left(\frac{Ain}{Ao}\right)^2\right]$$

$$Ks\ (eff) = Kss \left(\frac{Ain}{Ao}\right)^2 + Ka \left[1 - \left(\frac{Ain}{Ao}\right)^2\right]$$

$$Cp\ (eff) = Rhos \cdot Cps \left(\frac{Ain}{Ao}\right)^2 + Rhoa \cdot Cpa \left[1 - \left(\frac{Ain}{Ao}\right)^2\right] .$$

Reference Tables A-2 and A-3 for term definitions.

G) Three main cases are treated:

i) A translating infinite rod in a three-zone (hot, adiabatic, and cold) furnace.

ii) A motionless rod with finite length inserted into the hot zone and infinite length in the cold zone. An adiabatic zone is included.

iii) A motionless infinite rod in a four-zone [hot, booster (optional), adiabatic, and cold] furnace.

COMPUTER PROGRAM

A flow diagram and complete program listing are given in Appendix A. Key program symbols are listed in Table A-1. The program is coded in BASIC language for a Hewlett-Packard (H-P) 9835 computer with printer/plotter output and occupies core storage of approximately 18 K.

Data are read in via the interactive mode on the keyboard with the required units specified. The general input is listed in Table A-2.

SELCAS contains an interactive case selection allowing for any one of the following.

Case I: Calculates and plots temperature profiles in a translating infinite rod. Reference pages 5 to 8 of the Thermal Model (Appendix B). Additional required input for this case is listed in Table A-3. The output consists of:

A) Input

B) Effective Conductivities

C) Peclet Numbers

D) Heat transfer coefficients and Biot numbers

E) Coefficients used in temperature calculations

F) Interface position and gradients in the liquid and solid at the interface

G) Tabulated temperature profiles in the sample.

NOTE: After the profiles are printed, the temperature at both ends of the adiabatic zone ($x = \pm 1/2$ zone length) should be checked as to the accuracy of the input values of Tla and Tsa. An interactive option is given to i) correct these input temperatures to agree with the printed profiles or ii) continue the program and plot the profiles. These temperatures (Tla and Tsa) at the outer edges of the adiabatic zone are used to calculate the radiative heat transfer coefficients. Page 14 of the Thermal Model in Appendix B should be referenced as to their importance.

H) Plot of temperature versus distance in the sample.

NOTE: In output G and H, x will be in the range $\text{Lim} \le x \le \text{Lim}$ where Lim is an input value. Fifty-one values are printed/plotted.

Case II: Calculates and plots the temperature profiles in a motionless rod with a finite length inserted into the hot zone. This case can be used to investigate the end effects which are not included in Case I or III. Reference pages 8 to 10 of the Thermal Model (Appendix B). Additional required input is given in Table A-4. The output is the same as for Case I except no Peclet numbers are printed.

Case III: Calculates and plots temperature profiles in an infinite motionless rod where an optional booster (tickler) heater has been added to the hot end. This case can be used to investigate interface position and gradients in the steady state mode with or without the booster heater. Reference pages 11 and 12 of the Thermal Model (Appendix B). Additional required input is listed in Table A-5. Output has the same format as Case II.

Case IV: Calculates the optimum cold end temperature (Tc) which will center the T_{Melt} isotherm within 10^{-6} cm of the center of the adiabatic zone. The hot end temperature (Th) is input. The interface position Xo [equation (39)] is set equal 0 and equations (38) and (39) solved simultaneously for Tc. Reference page 12 in Thermal Model (Appendix B). Temperature profiles are then calculated from Case III equations. This case is of interest to crystal growers desiring the melt interface in the middle of the adiabatic zone. In many cases this position is the optimum for the flattest possible interface. Additional required input is the same as Case III (Table A-5).

NOTE: The solution for Tc involves an iteration between that equation and the Biot number calculation. If the solution cannot be found within 10 iterations an error message is printed and an option to select another case is given. The output has the same format as Case III with the calculated Tc being printed also.

Case V: Calculates the optimum length for the adiabatic zone in order to achieve a designated liquid gradient at the solid-liquid interface. The booster (tickler) heater may be on or off. Equation (38) of the Thermal Model is solved for the adiabatic zone length La. Reference page 12 of the Thermal Model (Appendix B). Additional required input is listed in Table A-6. The output has the same format as Case I parts A, B, and D plus the calculated adiabatic zone length.

NOTE: If the calculated adiabatic zone length is negative this implies the designated liquid gradient cannot be achieved. An interactive option is given to calculate Case III temperature profiles.

The subroutine BIOTCAL calculates the radiative and conductive heat transfer coefficients. These plus the input convective heat transfer coefficients are used to compute effective heat transfer coefficients for the hot and cold zones of the furnace.

$$H_H \text{ (eff)} = H_H \text{ rad} + H_H \text{ conv} + H_H \text{ cond}$$

$$H_C \text{ (eff)} = H_C \text{ rad} + H_C \text{ conv} + H_C \text{ cond}$$

These effective values are in turn used to calculate the Biot numbers. Reference pages 12 to 15 and page 24 of the Thermal Model (Appendix B). If the Biot numbers are available as input they should be set in this section.

TXPLOT controls the plotting of temperature versus distance in the sample. AXE and LABLER subroutines are called from here. These are H-P 9835 utility subroutines which draw and label the axes and would probably require changing if the program is run on another computer. The "Plotter is" statement should be checked for correct set-up even if running on the H-P 9835.

SAMPLE PROBLEMS

Each of the five cases was run for a 0.5 cm radius Mn-Bi/Bi eutectic sample. The sample was enclosed in a 0.6-cm radius fused silica ampoule. Furnace configuration was modeled with the Solidification Experiment System (SES) furnace developed by TRW for use on the Space Shuttle. Forced convection with helium gas is used for heat extraction in the cold end; stagnant helium gas is in the furnace cavity in the hot end.

In Cases III and IV the booster heater was not turned on, and Tb = Th was used to model this. Case V did utilize the booster heater. The general input for each case was the same and is listed in Table A-7. The specific case input is listed in Table A-8. All output from the five cases follow the Concluding Remarks section.

CONCLUDING REMARKS

Current work is being devoted to:

A) Attempting to evaluate furnace performance by using this model along with temperature data from a well characterized and instrumented sample[1] to solve for effective heat transfer coefficients.

B) Compiling a users guide to accompany the computer program for R. J. Naumann's "An Analytical Approach to Thermal Modeling of Bridgman-Type Crystal Growth: Two Dimensional Analysis."

Both tasks will be the subject of a further report.

1. Data from NASA's SPAR 9 flight. Mn-Bi/Bi Solidification Experiment.

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1-D MODEL OF CRYSTAL GROWTH
SAMPLE CASE I

TEMPERATURE OF HOT ZONE (C)	450
TEMPERATURE OF INTERFACE (C)	271.5
TEMPERATURE OF COLD ZONE (C)	40
CONDUCTIVITY OF LIQUID (W/cm-C)	.124
CONDUCTIVITY OF SOLID (W/cm-C)	.072
CONVECTIVE HEAT TRANSFER COEFF.-HOT END (W/cm2-C)	0
CONVECTIVE HEAT TRANSFER COEFF.-COLD END(W/cm2-C)	.0312
CONDUCTIVITY OF GAS - HOT END (W/cm-C)	.003
CONDUCTIVITY OF GAS - COLD END (W/cm-C)	0
CONDUCTIVITY OF AMPOULE (W/cm-C)	.02
SAMPLE RADIUS (cm)	.5
AMPOULE OUTER RADIUS (cm)	.6
INSIDE RADIUS OF FURNACE MUFFLE IN HOT ZONE(cm)	2.6
INSIDE RADIUS OF FURNACE MUFFLE IN COLD ZONE(cm)	1.77
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-HOT END-	.7695
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-COLD END-	.9486
EMISSIVITY OF FURNACE -HOT END	.3
EMISSIVITY OF FURNACE -COLD END	.3
LENGTH OF ADIABATIC ZONE (cm)	2.03
TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE (C)	327
TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE (C)	133
CALCULATED EFFECTIVE CONDUCTIVITY OF LIQUID (W/cm-C)	9.22222222223E-02
CALCULATED EFFECTIVE CONDUCTIVITY OF SOLID (W/cm-C)	5.61111111112E-02

CASE I

AVERAGE SAMPLE DENSITY (g/cm3)	10.05
AVERAGE AMPOULE DENSITY (g/cm3)	2.3
AVERAGE SAMPLE SPECIFIC HEAT (W-sec/g-C)	.1463
AVERAGE AMPOULE SPECIFIC HEAT (W-sec/g-C)	.493
AMPOULE VELOCITY (Cm/sec)	.0028
HEAT OF FUSION (W-sec/g)	50.16
CALCULATED PECLEC NO. FOR THE LIQUID	2.49119584337E-02
CALCULATED PECLEC NO. FOR THE SOLID	4.09444069307E-02

CALCULATED EMISSIVITY FUNCTION (Feh)-HOT	.544067658338
CALCULATED EMISSIVITY FUNCTION (Fec)-COLD	.541962660261
CALCULATED RADIATIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	4.11201340730E-03
CALCULATED RADIATIVE HEAT TRANS. COEFF.-COLD (W/Cm2-C)	4.72619886225E-04
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	3.40985719206E-03
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	0
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-HOT(W/cm2-C)	7.52187059936E-03
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	3.16726198862E-02
CALCULATED BIOT NO. -HOT END-	4.89374713693E-02
CALCULATED BIOT NO. -COLD END-	.338677519574

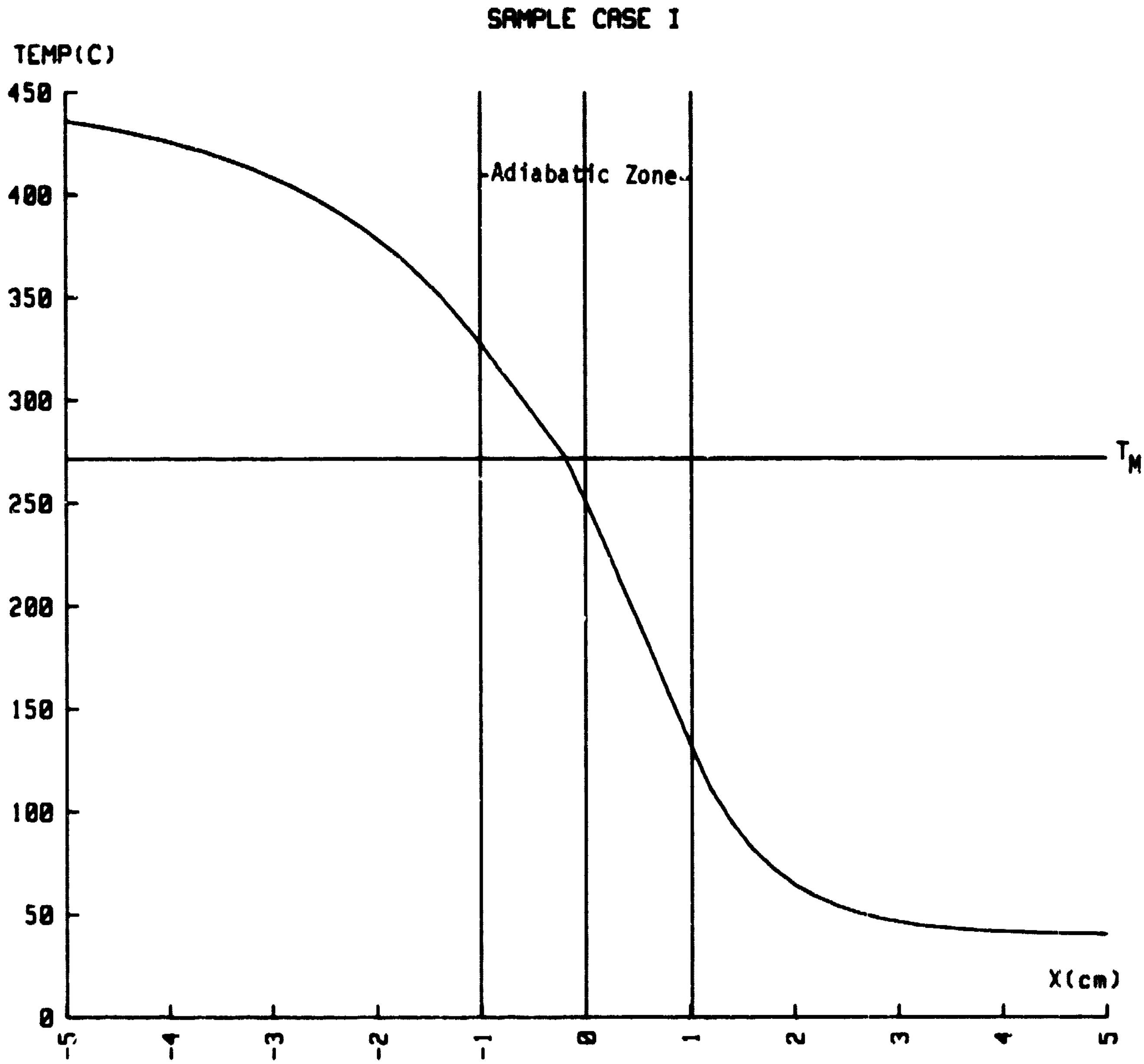
THE FOLLOWING COEFFICIENTS ARE USED IN CALCULATING TEMPERATURE
A= 1923.32846936 B=-1664.08424353 ASTAR= 1923.32846973 BSTAR=-1672.01967207 C=
91.3925254013 D= 122.083895174

INTERFACE POSITION Xo (cm)	-.178038124795
GRADIENT IN LIQUID AT Xo (deg C/cm)	-69.5838036l4
GRADIENT IN SOLID AT Xo (deg C/cm)	-112.721895074

TEMPERATURE PROFILE

X(cm)	T(C)
-5	435.951856441
-4.8	434.341590689
-4.6	432.546748534
-4.4	430.546172943
-4.2	428.31628176
-4	425.83078973
-3.8	423.060398653
-3.6	419.972452034
-3.4	416.530550126
-3.2	412.694120874
-3	408.417941658
-2.8	403.651606221
-2.6	398.338930504
-2.4	392.417290353
-2.2	385.81688334
-2	378.459905943
-1.8	370.259636433
-1.6	361.1194126
-1.4	350.931492371
-1.2	339.575783746
-1	326.92217423
-.8	313.6104447
-.6	300.1877146
-.4	286.65305831
-.2	273.00554233
0	251.30879766
.2	228.33241068
.4	205.04028899
.6	181.428094117
.8	157.4914277
1	133.22583079
1.2	111.352633473
1.4	94.6000530217
1.6	81.7807394768
1.8	71.9712178767
2	64.4648320074
2.2	58.7208384589
2.4	54.3254526522
2.6	50.9620407315
2.8	48.3883099483
3	46.418854437
3.2	44.9117989842
3.4	43.7585786526
3.6	42.8761180033
3.8	42.2008465258
4	41.684119158
4.2	41.2887120047
4.4	40.9861408103
4.6	40.7546090159
4.8	40.577437584
5	40.4418634768

Input temperatures at hot and cold edge of adiabatic zone were checked and program continued.


SAMPLE CASE I
TEMP(C)
450
400
350
300
250
200
150
100
50
0
Adiabatic Zone
T_M
X(cm)
-5
-4
-3
-2
-1
0
1
2
3
4
5

1-D MODEL OF CRYSTAL GROWTH
SAMPLE CASE II

TEMPERATURE OF HOT ZONE (C)	450
TEMPERATURE OF INTERFACE (C)	271.5
TEMPERATURE OF COLD ZONE (C)	40
CONDUCTIVITY OF LIQUID (W/cm-C)	.124
CONDUCTIVITY OF SOLID (W/cm-C)	.072
CONVECTIVE HEAT TRANSFER COEFF.-HOT END (W/cm2-C)	0
CONVECTIVE HEAT TRANSFER COEFF.-COLD END(W/cm2-C)	.0312
CONDUCTIVITY OF GAS - HOT END (W/cm-C)	.003
CONDUCTIVITY OF GAS - COLD END (W/cm-C)	0
CONDUCTIVITY OF AMPOULE (W/cm-C)	.02
SAMPLE RADIUS (cm)	.5
AMPOULE OUTER RADIUS (cm)	.6
INSIDE RADIUS OF FURNACE MUFFLE IN HOT ZONE(cm)	2.6
INSIDE RADIUS OF FURNACE MUFFLE IN COLD ZONE(cm)	1.77
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-HOT END-	.7695
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-COLD END-	.9486
EMISSIVITY OF FURNACE -HOT END	.3
EMISSIVITY OF FURNACE -COLD END	.3
LENGTH OF ADIABATIC ZONE (cm)	2.03
TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE (C)	327
TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE (C)	133
CALCULATED EFFECTIVE CONDUCTIVITY OF LIQUID (W/cm-C)	9.22222222223E-02
CALCULATED EFFECTIVE CONDUCTIVITY OF SOLID (W/cm-C)	5.61111111112E-02

CASE II

BIOT NO. AT END OF ROD IN HOT ZONE	.0507
LENGTH OF AMPOULE INSERTED INTO HOT ZONE (cm)	2.5

CALCULATED EMISSIVITY FUNCTION (Feh)-HOT	.544067658338
CALCULATED EMISSIVITY FUNCTION (Fec)-COLD	.541962660261
CALCULATED RADIATIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	4.11201340730E-03
CALCULATED RADIATIVE HEAT TRANS. COEFF.-COLD (W/Cm2-C)	4.72619886225E-04
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	3.40985719206E-03
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	0
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-HOT(W/cm2-C)	7.52187059936E-03
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	3.16726198862E-02
CALCULATED BIOT NO. -HOT END-	4.89374713693E-02
CALCULATED BIOT NO. -COLD END-	.338677519574

THE FOLLOWING COEFFICIENTS ARE USED IN CALCULATING TEMPERATURE
B=-2.43982292246 C= 78.2141450111 D= 1[illegible].221897134

INTERFACE POSITION Xo (cm)	-.41376185103
GRADIENT IN LIQUID AT Xo (deg C/cm)	-65.2762986338
GRADIENT IN SOLID AT Xo (deg C/cm)	-107.235797755

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TEMPERATURE PROFILE

X(cm)	T(C)
-2	359.134587772
-1.92	356.244814424
-1.84	353.191883499
-1.76	349.970482121
-1.68	346.575004245
-1.6	342.999540885
-1.52	339.23786984
-1.44	335.283444853
-1.36	331.12938423
-1.28	326.768458865
-1.2	322.193079653
-1.12	317.39528428
-1.04	312.366727385
-.96	307.156404538
-.88	301.934300647
-.8	296.712196756
-.72	291.490092865
-.64	286.267988975
-.56	281.045885084
-.48	275.823781193
-.4	270.023548834
-.32	261.440685014
-.24	252.857821193
-.16	244.274957373
-.08	235.692093552
0	227.109229732
.08	218.526365912
.16	209.943502091
.24	201.360638271
.32	192.77777445
.4	184.19491063
.48	175.61204681
.56	167.029182989
.64	158.446319169
.72	149.863455349
.8	141.280591528
.88	132.697727708
.96	124.114863888
1.04	115.577467354
1.12	107.722789311
1.2	100.684438796
1.28	94.3775758408
1.36	88.7261778013
1.44	83.662122965
1.52	79.1243694444
1.6	75.0582193543
1.68	71.414659502
1.76	68.1497705755
1.84	65.2241977475
1.92	62.6026762923
2	60.2536065042

Input temperatures at hot and cold edge of adiabatic zone were checked. They varied from the profile. When the interactive mode allowed for a correction the following was made:

Tla = 310°

Tsa = 113°

The following run uses this new input.

1 D MODEL OF CRYSTAL GROWTH
SAMPLE CASE II

TEMPERATURE OF HOT ZONE (C)	450
TEMPERATURE OF INTERFACE (C)	271.5
TEMPERATURE OF COLD ZONE (C)	40

CONDUCTIVITY OF LIQUID (W/cm-C)	.124
CONDUCTIVITY OF SOLID (W/cm-C)	.072
CONVECTIVE HEAT TRANSFER COEFF.-HOT END (W/cm2-C)	0
CONVECTIVE HEAT TRANSFER COEFF.-COLD END(W/cm2-C)	.0312
CONDUCTIVITY OF GAS - HOT END (W/cm-C)	.003
CONDUCTIVITY OF GAS - COLD END (W/cm-C)	0
CONDUCTIVITY OF AMPOULE (W/cm-C)	.02
SAMPLE RADIUS (cm)	.5
AMPOULE OUTER RADIUS (cm)	.6
INSIDE RADIUS OF FURNACE MUFFLE IN HOT ZONE(cm)	2.6
INSIDE RADIUS OF FURNACE MUFFLE IN COLD ZONE(cm)	1.77
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-HOT END-	.7695
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-COLD END-	.9486
EMISSIVITY OF FURNACE -HOT END	.3
EMISSIVITY OF FURNACE -COLD END	.3
LENGTH OF ADIABATIC ZONE (cm)	2.03
TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE (C)	310
TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE (C)	119
CALCULATED EFFECTIVE CONDUCTIVITY OF LIQUID (W/cm-C)	9.22222222223E-02
CALCULATED EFFECTIVE CONDUCTIVITY OF SOLID (W/cm-C)	5.61111111112E-02

CASE II

BIOT NO. AT END OF ROD IN HOT ZONE	.0507
LENGTH OF AMPOULE INSERTED INTO HOT ZONE (cm)	2.5

CALCULATED EMISSIVITY FUNCTION (Feh)-HOT	.544067658338
CALCULATED EMISSIVITY FUNCTION (Fec)-COLD	.541962660261
CALCULATED RADIATIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	4.04238828752E-03
CALCULATED RADIATIVE HEAT TRANS. COEFF.-COLD (W/Cm2-C)	4.56648445440E-04
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	3.40985719206E-03
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	0
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-HOT(W/cm2-C)	7.45224547958E-03
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	3.16566484454E-02
CALCULATED BIOT NO. -HOT END-	4.84844886623E-02
CALCULATED BIOT NO. -COLD END-	.338506735851

THE FOLLOWING COEFFICIENTS ARE USED IN CALCULATING TEMPERATURE
B=-2.48447502180 C= 78.0336904002 D= 132.577142304

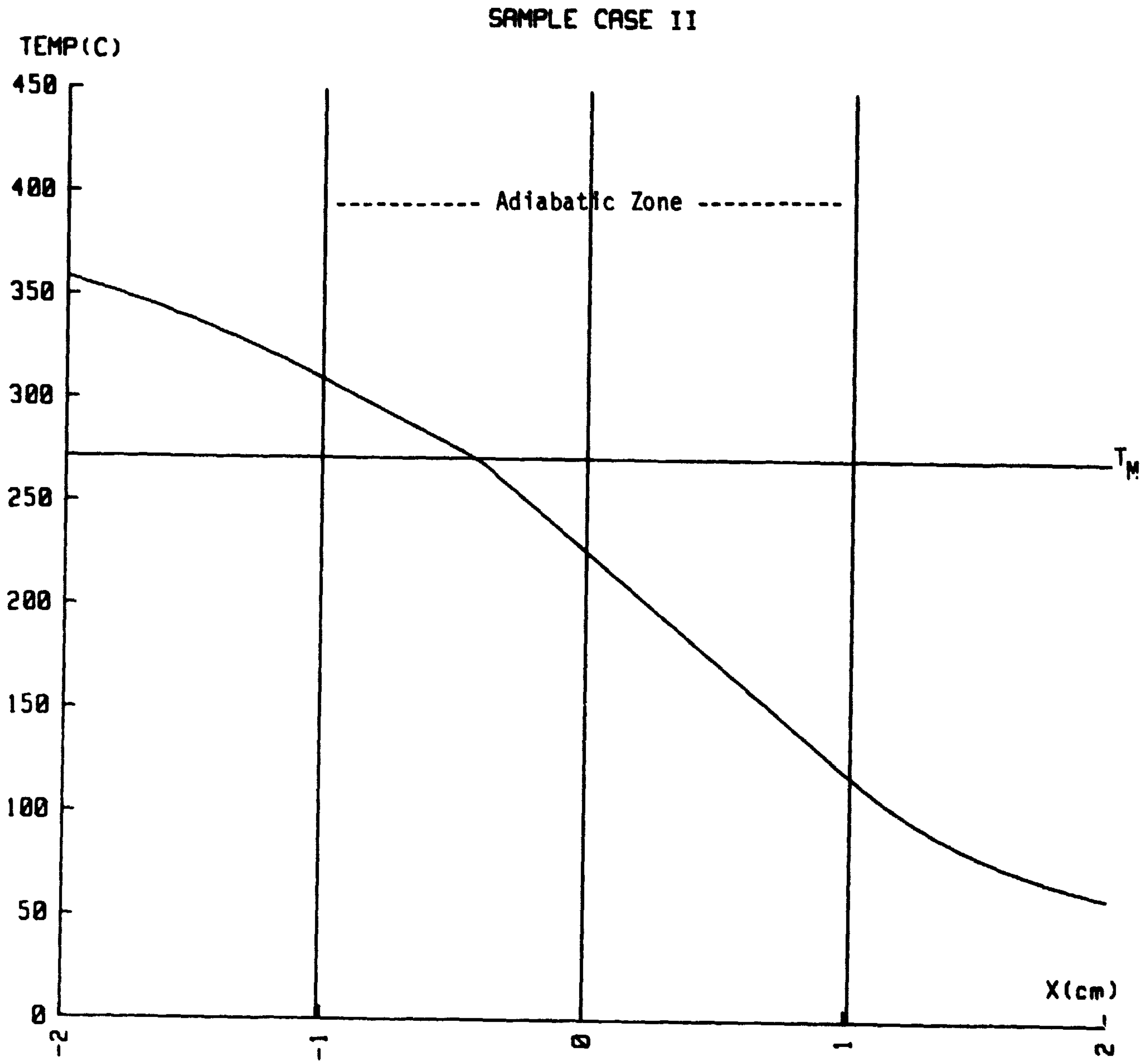
INTERFACE POSITION Xo (cm)	-.419113415946
GRADIENT IN LIQUID AT Xo (deg C/cm)	-65.109271623
GRADIENT IN SOLID AT Xo (deg C/cm)	-107.011278113

TEMPERATURE PROFILE

X(cm)	T(C)
-2	358.604688279
-1.92	355.71687064
-1.84	352.666495634
-1.76	349.448303983
-1.68	346.056747072
-1.6	342.485977374
-1.52	338.72983839
-1.44	334.781854
-1.36	330.635217328
-1.28	326.28277899
-1.2	321.717034768
-1.12	316.930112676
-1.04	311.91375939

-.96	306.716731518
-.88	301.507989788
-.8	296.299248058
-.72	291.090506329
-.64	285.881764599
-.56	280.673022869
-.48	275.464281139
-.4	269.45464893
-.32	260.893746681
-.24	252.332844432
-.16	243.771942183
-.08	235.211039934
0	226.650137685
.08	218.089235436
.16	209.528333187
.24	200.967430938
.32	192.406528689
.4	183.84562644
.48	175.284724191
.56	166.723821942
.64	158.162919692
.72	149.602017444
.8	141.041115195
.88	132.480212945
.96	123.919310697
1.04	115.403748088
1.12	107.56899419
1.2	100.54830286
1.28	94.2570897066
1.36	88.6195590011
1.44	83.5677905018
1.52	79.0409211469
1.6	74.984411797
1.68	71.3493901474
1.76	68.0920619269
1.84	65.1731832614
1.92	62.5575878739
2	60.2137634087

Input Tla and Tsa were checked and program allowed to continue.


SAMPLE CASE II
TEMP(C)
450
400
350
300
250
200
150
100
50
0
Adiabatic Zone
T_M
X(cm)
-2
-1
0
1
2

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1-D MODEL OF CRYSTAL GROWTH
SAMPLE CASE III

TEMPERATURE OF HOT ZONE (C)	450
TEMPERATURE OF INTERFACE (C)	271.5
TEMPERATURE OF COLD ZONE (C)	40
CONDUCTIVITY OF LIQUID (W/cm-C)	.124
CONDUCTIVITY OF SOLID (W/cm-C)	.072
CONVECTIVE HEAT TRANSFER COEFF.-HOT END (W/cm2-C)	0
CONVECTIVE HEAT TRANSFER COEFF.-COLD END(W/cm2-C)	.0312
CONDUCTIVITY OF GAS - HOT END (W/cm-C)	.003
CONDUCTIVITY OF GAS - COLD END (W/cm-C)	0
CONDUCTIVITY OF AMPOULE (W/cm-C)	.02
SAMPLE RADIUS (cm)	.5
AMPOULE OUTER RADIUS (cm)	.6
INSIDE RADIUS OF FURNACE MUFFLE IN HOT ZONE(cm)	2.6
INSIDE RADIUS OF FURNACE MUFFLE IN COLD ZONE(cm)	1.77
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-HOT END-	.7695
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-COLD END-	.9486
EMISSIVITY OF FURNACE -HOT END	.3
EMISSIVITY OF FURNACE -COLD END	.3
LENGTH OF ADIABATIC ZONE (cm)	2.03
TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE (C)	327
TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE (C)	133
CALCULATED EFFECTIVE CONDUCTIVITY OF LIQUID (W/cm-C)	9.22222222223E-02
CALCULATED EFFECTIVE CONDUCTIVITY OF SOLID (W/cm-C)	5.61111111112E-02

CASE III

TEMPERATURE OF TICKLER HEATER (C)	450
LENGTH OF TICKLER HEATER (cm)	0

CALCULATED EMISSIVITY FUNCTION (Feh)-HOT	.544067658338
CALCULATED EMISSIVITY FUNCTION (Fec)-COLD	.541962660261
CALCULATED RADIATIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	4.11201340730E-03
CALCULATED RADIATIVE HEAT TRANS. COEFF.-COLD (W/Cm2-C)	4.72619886225E-04
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	3.40985719206E-03
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	0
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-HOT(W/cm2-C)	7.52187059936E-03
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	3.16726198862E-02
CALCULATED BIOT NO. -HOT END-	4.89374713693E-02
CALCULATED BIOT NO. -COLD END-	.338677519574

THE FOLLOWING COEFFICIENTS ARE USED IN CALCULATING TEMPERATURE
A=-130.957228179 B= 0 C= 81.8170404875 D= 130.957228179

INTERFACE POSITION Xo (cm)	-.318741494102	
GRADIENT IN LIQUID AT Xo (deg C/cm)		-68.283218687
GRADIENT IN SOLID AT Xo (deg C/cm)		-112.227864377

TEMPERATURE PROFILE

X(cm)	T(C)
-5	433.604166315
-4.8	431.802021864
-4.6	429.801795101
-4.4	427.581713854
-4.2	425.117612864
-4	422.382670759

-3.8	419.347118092
-3.6	415.977913321
-3.4	412.238383152
-3.2	408.087823344
-3	403.48105567
-2.8	398.367936141
-2.6	392.692809199
-2.4	386.393901934
-2.2	379.40265166
-2	371.642959655
-1.8	363.030362802
-1.6	353.471114267
-1.4	342.861163034
-1.2	331.085021341
-1	318.018523541
-.8	304.361879804
-.6	290.705236066
-.4	277.048592329
-.2	258.173895704
0	235.728322829
.2	213.282749954
.4	190.837177078
.6	168.391604203
.8	145.946031328
1	123.500458452
1.2	103.479837122
1.4	88.2494159627
1.6	76.6731586969
1.8	67.8743388284
2	61.1865787593
2.2	56.1033817634
2.4	52.2397725065
2.6	49.3031409932
2.8	47.0710817782
3	45.3745501169
3.2	44.0850593821
3.4	43.104950143
3.6	42.3599939413
3.8	41.7937716055
4	41.363400353
4.2	41.0362860672
4.4	40.7876547858
4.6	40.5986764478
4.8	40.4550388008
5	40.3458634643

Input Tla and Tsa checked. The following corrections were made:

Tla = 318°
Tsa = 123°

Next case uses these values.

1-D MODEL OF CRYSTAL GROWTH
SAMPLE CASE III

TEMPERATURE OF HOT ZONE (C)	450
TEMPERATURE OF INTERFACE (C)	271.5
TEMPERATURE OF COLD ZONE (C)	40
CONDUCTIVITY OF LIQUID (W/cm-C)	.124
CONDUCTIVITY OF SOLID (W/cm-C)	.072
CONVECTIVE HEAT TRANSFER COEFF.-HOT END (W/cm2-C)	0
CONVECTIVE HEAT TRANSFER COEFF.-COLD END(W/cm2-C)	.0312
CONDUCTIVITY OF GAS - HOT END (W/cm-C)	.003
CONDUCTIVITY OF GAS - COLD END (W/cm-C)	0
CONDUCTIVITY OF AMPOULE (W/cm-C)	.02
SAMPLE RADIUS (cm)	.5

AMPOULE OUTER RADIUS (cm)	.6
INSIDE RADIUS OF FURNACE MUFFLE IN HOT ZONE(cm)	2.6
INSIDE RADIUS OF FURNACE MUFFLE IN COLD ZONE(cm)	1.77
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-HOT END-	.7695
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-COLD END-	.9486
EMISSIVITY OF FURNACE -HOT END	.3
EMISSIVITY OF FURNACE -COLD END	.3
LENGTH OF ADIABATIC ZONE (cm)	2.03
TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE (C)	318
TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE (C)	123
CALCULATED EFFECTIVE CONDUCTIVITY OF LIQUID (W/cm-C)	9.22222222223E-02
CALCULATED EFFECTIVE CONDUCTIVITY OF SOLID (W/cm-C)	5.61111111112E-02

CASE III

TEMPERATURE OF TICKLER HEATER (C)	450
LENGTH OF TICKLER HEATER (cm)	0

CALCULATED EMISSIVITY FUNCTION (Feh)-HOT	.544067658338
CALCULATED EMISSIVITY FUNCTION (Fec)-COLD	.541962660261
CALCULATED RADIATIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	4.07496086894E-03
CALCULATED RADIATIVE HEAT TRANS. COEFF.-COLD (W/Cm2-C)	4.61152580853E-04
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	3.40985719206E-03
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	0
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-HOT(W/cm2-C)	.007484818061
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	3.16611525809E-02
CALCULATED BIOT NO. -HOT END-	4.86964066619E-02
CALCULATED BIOT NO. -COLD END-	.338554898884

THE FOLLOWING COEFFICIENTS ARE USED IN CALCULATING TEMPERATURE
A=-131.14432183 B= 0 C= 81.7466779081 D= 131.14432183

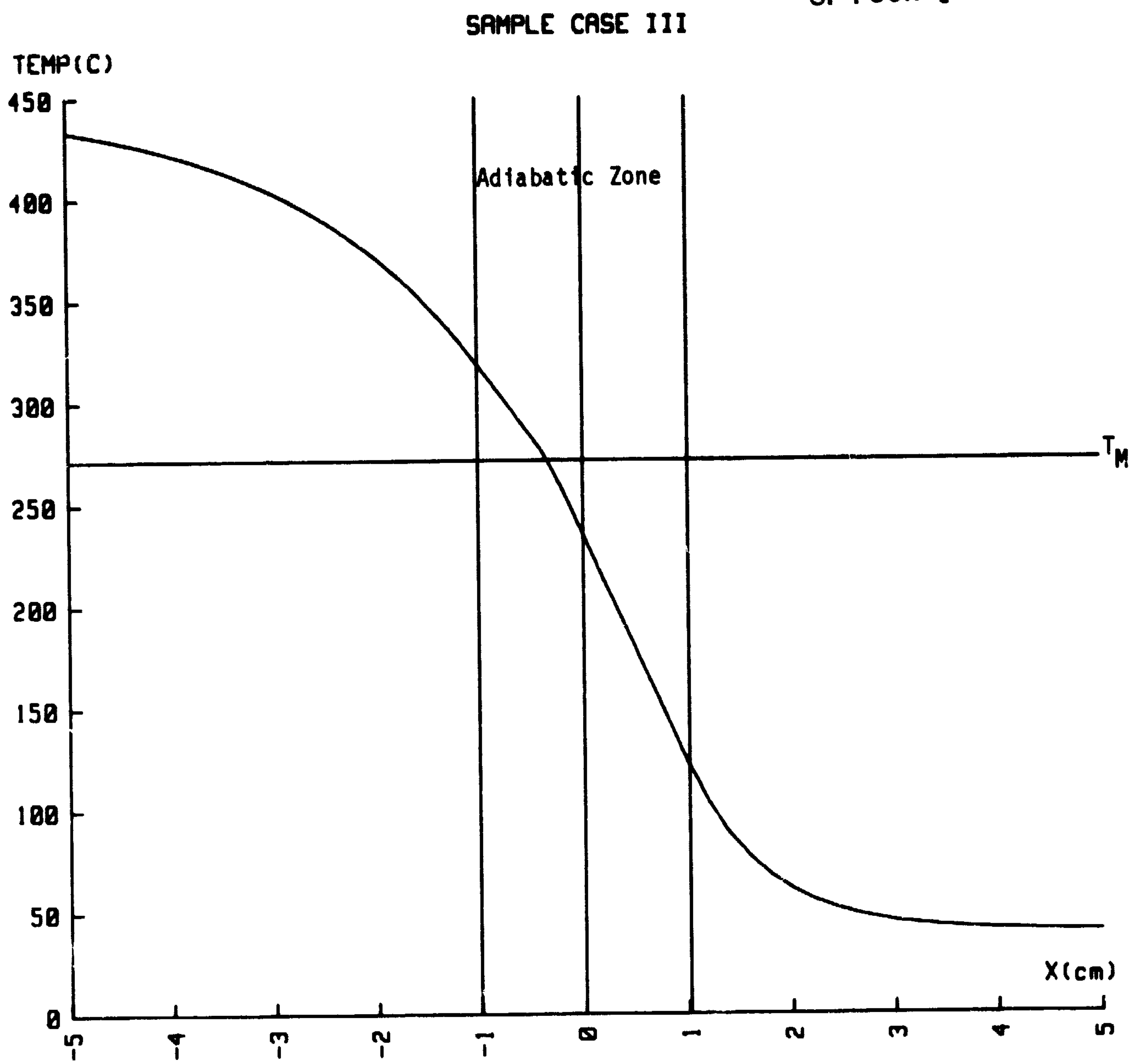
INTERFACE POSITION Xo (cm)	-.320758831802	
GRADIENT IN LIQUID AT Xo (deg C/cm)		-68.2121434732
GRADIENT IN SOLID AT Xo (deg C/cm)		-112.111047689

TEMPERATURE PROFILE

X(cm)	T(C)
-5	433.496393694
-4.8	431.687113483
-4.6	429.679482996
-4.4	427.451757213
-4.2	424.979807222
-4	422.236858874
-3.8	419.193202786
-3.6	415.815872551
-3.4	412.068287681
-3.2	407.909857386
-3	403.295540935
-2.8	398.175359809
-2.6	392.493856374
-2.4	386.18949321
-2.2	379.193986592
-2	371.431566887
-1.8	362.818157877
-1.6	353.260466137
-1.4	342.654970534
-1.2	330.886800966
-1	317.832496018
-.8	304.190067323

.6	290.547638629
-.4	276.905209934
-.2	257.961600849
0	235.539391311
.2	213.117181773
.4	190.694972235
.6	168.272762698
.8	145.85055316
1	123.428343622
1.2	103.428158508
1.4	88.2125309016
1.6	76.6469434178
1.8	67.8557967573
2	61.1735370149
2.2	56.0942684076
2.4	52.2334532674
2.6	49.2987997379
2.8	47.0681331486
3	45.3725757751
3.2	44.0837615609
3.4	43.1041178725
3.6	42.3594785403
3.8	41.7934689374
4	41.3632380097
4.2	41.0362141393
4.4	40.7876392345
4.6	40.5986943626
4.8	40.4550750193
5	40.3459081731

Input Tla and Tsa were checked and program allowed to continue.


SAMPLE CASE III
TEMP(C)
450
400
350
300
250
200
150
100
50
0
Adiabatic Zone
T_M
X(cm)
-5
-4
-3
-2
-1
0
1
2
3
4
5

1-D MODEL OF CRYSTAL GROWTH
SAMPLE CASE IV

TEMPERATURE OF HOT ZONE (C)	450
TEMPERATURE OF INTERFACE (C)	271.5
TEMPERATURE OF COLD ZONE (C)	40
CONDUCTIVITY OF LIQUID (W/cm-C)	.124
CONDUCTIVITY OF SOLID (W/cm-C)	.072
CONVECTIVE HEAT TRANSFER COEFF.-HOT END (W/cm2-C)	0
CONVECTIVE HEAT TRANSFER COEFF.-COLD END(W/cm2-C)	.0312
CONDUCTIVITY OF GAS - HOT END (W/cm-C)	.003
CONDUCTIVITY OF GAS - COLD END (W/cm-C)	0
CONDUCTIVITY OF AMPOULE (W/cm-C)	.02
SAMPLE RADIUS (cm)	.5
AMPOULE OUTER RADIUS (cm)	.6
INSIDE RADIUS OF FURNACE MUFFLE IN HOT ZONE(cm)	2.6
INSIDE RADIUS OF FURNACE MUFFLE IN COLD ZONE(cm)	1.77
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-HOT END-	.7695
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-COLD END-	.9486
EMISSIVITY OF FURNACE -HOT END	.3
EMISSIVITY OF FURNACE -COLD END	.3
LENGTH OF ADIABATIC ZONE (cm)	2.03
TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE (C)	327
TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE (C)	133
CALCULATED EFFECTIVE CONDUCTIVITY OF LIQUID (W/cm-C)	9.22222222223E-02
CALCULATED EFFECTIVE CONDUCTIVITY OF SOLID (W/cm-C)	5.61111111112E-02

CASE IV   Tc CALCULATION

CALCULATED Tc(C)	97.270796601
TEMPERATURE OF TICKLER HEATER (C)	450
LENGTH OF TICKLER HEATER (cm)	1.8

CALCULATED EMISSIVITY FUNCTION (Feh)-HOT	.544067658338
CALCULATED EMISSIVITY FUNCTION (Fec)-COLD	.541962660261
CALCULATED RADIATIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	4.11201340730E-03
CALCULATED RADIATIVE HEAT TRANS. COEFF.-COLD (W/Cm2-C)	6.71110029012E-04
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	3.40985719206E-03
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	0
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-HOT(W/cm2-C)	7.52187059936E-03
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	.031871110029
CALCULATED BIOT NO. -HOT END-	4.89374713693E-02
CALCULATED BIOT NO. -COLD END-	.340799988428

THE FOLLOWING COEFFICIENTS ARE USED IN CALCULATING TEMPERATURE
A=-73.0062345341 B= 0 C= 72.6977544731 D= 45.6621749258

INTERFACE POSITION Xo (cm)	-2.85152250032E-08
GRADIENT IN LIQUID AT Xo (deg C/cm)	-60.8622235947
GRADIENT IN SOLID AT Xo (deg C/cm)	-100.030981353

TEMPERATURE PROFILE

X(cm)	T(C)
-5	435.38605949
4.8	433.779771434
4.6	431.996928581
-4.4	430.018124946

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-4.2	427.821821547
-4	425.384111942
-3.8	422.678462024
-3.6	419.675421188
-3.4	416.34230178
-3.2	412.642823287
-3	408.536717428
-2.8	403.979289848
-2.6	398.920933621
-2.4	393.306589278
-2.2	387.07514551
-2	380.158773977
-1.8	372.482190965
-1.6	363.961838068
-1.4	354.504972427
-1.2	344.008657485
-1	332.362221859
-.8	320.18977714
-.6	308.017332421
-.4	295.844887702
-.2	283.672442983
0	271.499997148
.2	251.493800877
.4	231.487604607
.6	211.481408336
.8	191.475212065
1	171.469015794
1.2	153.630440521
1.4	140.071582928
1.6	129.774680279
1.8	121.954979881
2	116.016522809
2.2	111.506724406
2.4	108.081881658
2.6	105.480978732
2.8	103.505794317
3	102.005794667
3.2	100.86666106
3.4	100.001577274
3.6	99.3446131116
3.8	98.8456996908
4	98.4668135724
4.2	98.179078898
4.4	97.9605666884
4.6	97.794623582
4.8	97.6686026396
5	97.5728994901

Input Tla and Tsa were checked. The following corrections were made:

Tla = 332°
Tsa = 171°

Next run uses this input.

1-D MODEL OF CRYSTAL GROWTH
SAMPLE CASE IV

TEMPERATURE OF HOT ZONE (C)	450
TEMPERATURE OF INTERFACE (C)	271.5
TEMPERATURE OF COLD ZONE (C)	97.270796601
CONDUCTIVITY OF LIQUID (W/cm-C)	.124
CONDUCTIVITY OF SOLID (W/cm-C)	.072
CONVECTIVE HEAT TRANSFER COEFF.-HOT END (W/cm2-C)	0
CONVECTIVE HEAT TRANSFER COEFF.-COLD END(W/cm2-C)	.0312
CONDUCTIVITY OF GAS - HOT END (W/cm-C)	.003
CONDUCTIVITY OF GAS - COLD END (W/cm-C)	0

CONDUCTIVITY OF AMPOULE (W/cm-C)	.02
SAMPLE RADIUS (cm)	.5
AMPOULE OUTER RADIUS (cm)	.6
INSIDE RADIUS OF FURNACE MUFFLE IN HOT ZONE(cm)	2.6
INSIDE RADIUS OF FURNACE MUFFLE IN COLD ZONE(cm)	1.77
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-HOT END-	.7695
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-COLD END-	.9486
EMISSIVITY OF FURNACE -HOT END	.3
EMISSIVITY OF FURNACE -COLD END	.3
LENGTH OF ADIABATIC ZONE (cm)	2.03
TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE (C)	332
TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE (C)	171
CALCULATED EFFECTIVE CONDUCTIVITY OF LIQUID (W/cm-C)	9.22222222223E-02
CALCULATED EFFECTIVE CONDUCTIVITY OF SOLID (W/cm-C)	5.61111111112E-02

CASE IV Tc CALCULATION

CALCULATED Tc(C)	97.175483728
TEMPERATURE OF TICKLER HEATER (C)	450
LENGTH OF TICKLER HEATER (cm)	1.8

CALCULATED EMISSIVITY FUNCTION (Feh)-HOT	.544067658338
CALCULATED EMISSIVITY FUNCTION (Fec)-COLD	.541962660261
CALCULATED RADIATIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	4.13278618099E-03
CALCULATED RADIATIVE HEAT TRANS. COEFF.-COLD (W/Cm2-C)	7.25332379524E-04
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	3.40985719206E-03
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	0
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-HOT(W/cm2-C)	7.54264337305E-03
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	3.19253323795E-02
CALCULATED BIOT NO. -HOT END-	4.90726195355E-02
CALCULATED BIOT NO. -COLD END-	.341379791 78

THE FOLLOWING COEFFICIENTS ARE USED IN CALCULATING TEMPERATURE
A=-72.9241498065 B= 0 C= 72.7015020313 D= 45.5813093083

INTERFACE POSITION Xo (cm)	1.28280063354E-08
GRADIENT IN LIQUID AT Xo (deg C/cm)	-60.9171141793
GRADIENT IN SOLID AT Xo (deg C/cm)	-100.121197562

TEMPFRATURE PROFILE

X(cm)	T(C)
5	435.43485571
-4.8	433.831604654
-4.6	432.05187653
-4.4	430.076245714
-4.2	427.883148313
-4	425.448646799
-3.8	422.746168734
3.6	419.746216734
-3.4	416.416046499
-3.2	412.719309425
3	408.615655841
-2.8	404.060294622
2.6	399.003504268
2.4	393.390090216
2.2	387.158782306
2	380.241566429
1.8	372.562941349
1.6	364.039095407

-1.4	354.576991338
-1.2	344.073350843
-1	332.417114961
-.8	320.233692124
-.6	308.050269289
-.4	295.866846453
-.2	283.683423617
0	271.500000781
.2	251.475761772
.4	231.451522259
.6	211.427282747
.8	191.403043235
1	171.378803722
1.2	153.525834788
1.4	139.959200417
1.6	129.658802454
1.8	121.838277827
2	115.900584382
2.2	111.392420913
2.4	107.969620789
2.6	105.370877[illegible]
2.8	103.3977944[illegible]
3	101.899741426
3.2	100.762352294
3.4	99.8987953961
3.6	99.2431442249
3.8	98.7453444165
4	98.3673924503
4.2	98.0604343474
4.4	97.8625628711
4.6	97.6971450637
4.8	97.571552437
5	97.4761968756

Input Tla and Tsa checked and program allowed to continue.

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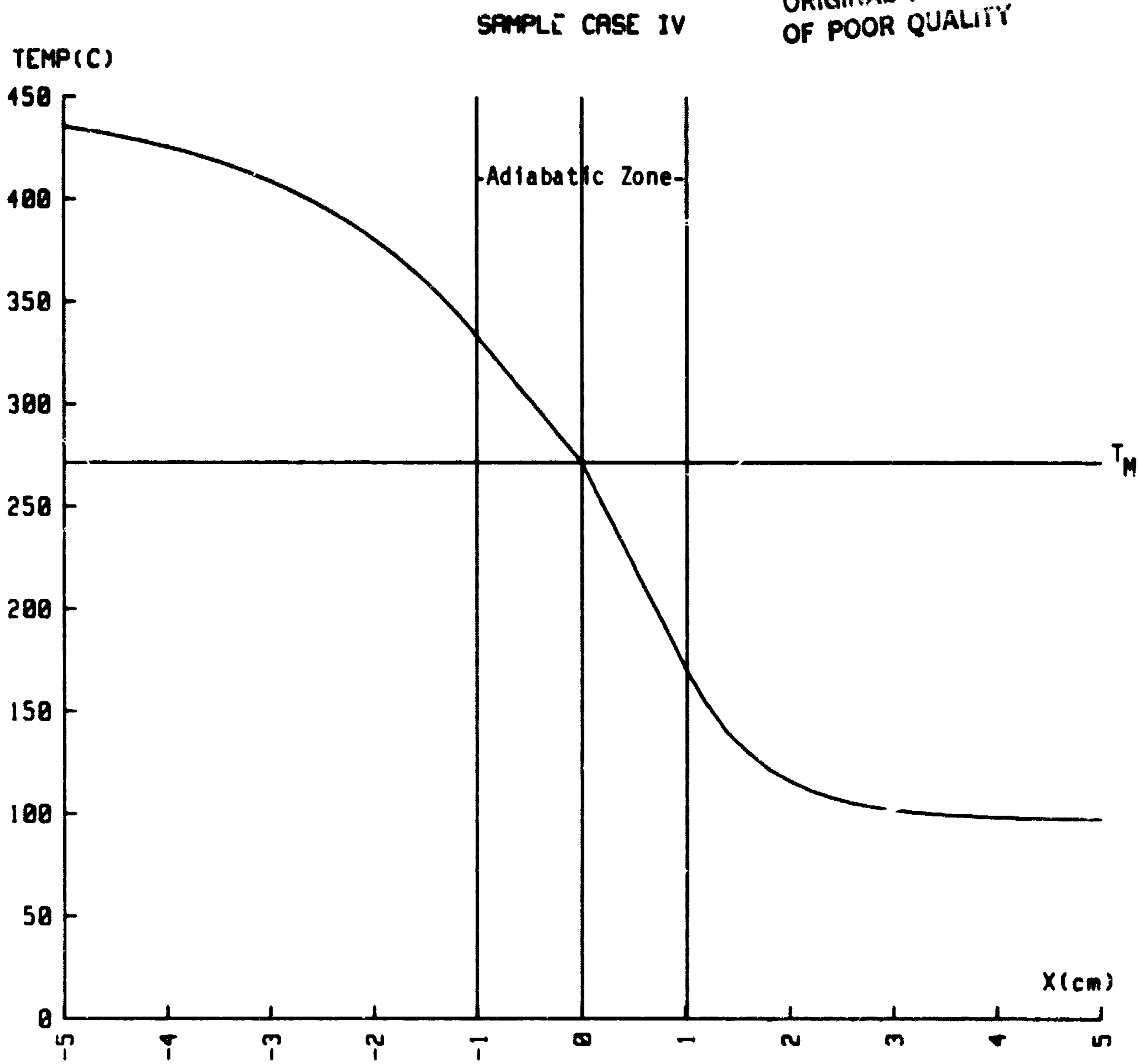

1-D MODEL OF CRYSTAL GROWTH
SAMPLE CASE V

TEMPERATURE OF HOT ZONE (C)	450
TEMPERATURE OF INTERFACE (C)	271.5
TEMPERATURE OF COLD ZONE (C)	40
CONDUCTIVITY OF LIQUID (W/cm-C)	.124
CONDUCTIVITY OF SOLID (W/cm-C)	.072
CONVECTIVE HEAT TRANSFER COEFF.-HOT END (W/cm2-C)	0
CONVECTIVE HEAT TRANSFER COEFF.-COLD END(W/cm2-C)	.0312
CONDUCTIVITY OF GAS - HOT END (W/cm-C)	.003
CONDUCTIVITY OF GAS - COLD END (W/cm-C)	0
CONDUCTIVITY OF AMPOULE (W/cm-C)	.02
SAMPLE RADIUS (cm)	.5
AMPOULE OUTER RADIUS (cm)	.6
INSIDE RADIUS OF FURNACE MUFFLE IN HOT ZONE(cm)	2.6
INSIDE RADIUS OF FURNACE MUFFLE IN COLD ZONE(cm)	1.77
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-HOT END-	.7695
EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-COLD END-	.9486
EMISSIVITY OF FURNACE -HOT END	.3
EMISSIVITY OF FURNACE -COLD END	.3
LENGTH OF ADIABATIC ZONE (cm)	2.03
TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE (C)	327
TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE (C)	133
CALCULATED EFFECTIVE CONDUCTIVITY OF LIQUID (W/cm-C)	9.22222222223E-02
CALCULATED EFFECTIVE CONDUCTIVITY OF SOLID (W/cm-C)	5.61111111112E-02

CASE V CALCULATES OPTIMUM La FOR GIVEN GRADIENT

TEMPERATURE OF TICKLER HEATER (C)	500
LENGTH OF TICKLER HEATER (cm)	1.8

CALCULATED EMISSIVITY FUNCTION (Feh)-HOT	.544067658338
CALCULATED EMISSIVITY FUNCTION (Fec)-COLD	.541962660261
CALCULATED RADIATIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	4.11201340730E-03
CALCULATED RADIATIVE HEAT TRANS. COEFF.-COLD (W/Cm2-C)	4.72619086225E-04
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)	3.40985719206E-03
CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	0
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-HOT(W/cm2-C)	7.52187059936E-03
CALCULATED EFFECTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)	3.16726198862E-02
CALCULATED BIOT NO. -HOT END-	4.89374713693E-02
CALCULATED BIOT NO. -COLD END-	.338677519574

FOR LIQUID GRADIENT = 85 (C/cm) AD. ZONE LENGTH= 1.46832791313 (cm)

NOTE: IF AD. ZONE LENGTH IS NEGATIVE--INPUT GRADIENT CANNOT BE ACHIEVED WITH GIVEN PARAMETERS.

NOTE: THE AD. ZONE LENGTH HAS BEEN CHANGED IN PROG. RUN CASE III FOR TEMP. PROFILES

APPENDIX A

TABLES, FLOW CHARTS, AND COMPUTER PROGRAM LISTINGS

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TABLES

TABLE A-1. KEY PROGRAM SYMBOLS

Computer Program Symbol	Thermal Model Notation
A	A
Af	a_f
Ain	inner radius of ampoule
Alfa	α
Ao	a_o
Aprime	A*
Astar	α*
B	B
Beta	β
Bh, Bc	B_i
Bhstar	β^*_H
Bprime	B*
Bstar	β*
C	C
Cps, Cpa	specific heat
D	D
Dhf	ΔH_f
Efhot, Efcold	ϵ, furnace
Ehot, Ecold	ϵ, sample/ampoule
Feh, Fec	Fe
Fl	F(L)
Gl	G_L
Glxo	$G_L(X_o)$
Gs	G_s
Gsxo	$G_s(X_o)$
Hcondh, Hcondc	H_{cond}
Hconvh, Hconvc	H_{conv}
Hradh, Hradc	H_{rad}
Hstarh, Hstarc	H*
Kgh, Kgc	k_G

TABLE A-1. (Concluded)

Computer Program Symbol	Thermal Model Notation
Kl, Kls	k_L
Ks, Kss	k_s
Ka	conductivity of ampoule
L	L
La	L_A
Lb, Lbt	L_B
Lf	L_f
Pl, Ps	P_e
Rhos, Rhoa	ρ
T	T
Tb	T_B
Tc	T_C
Th	T_H
Tla	$T_L(-X_1)$
Tm	T_M
To	T_o
Tostar	T_o
Tsa	$T_s(X_1)$
U	U
X	X
Xo	X_o
X1	X_1
X2	X_2
X3	X_3

TABLE A-2. GENERAL INPUT FOR ALL CASES

Variable	Units	Description
Id$		18 Character Run Identification
Th	°C	Temperature of Furnace Muffle - Hot Zone
Tm	°C	Melt Temperature of Sample
Tc	°C	Temperature of Furnace Muffle - Cold Zone
Kls	W/cm-°C	Conductivity of Sample Liquid
Kss	W/cm-°C	Conductivity of Sample Solid
Hconvh	W/cm^2-°C	Heat Transfer Coefficient due to Convection - Hot Zone
Hconvc	W/cm^2-°C	Heat Transfer Coefficient due to Convection - Cold Zone
Kgh	W/cm-°C	Conductivity of Gas in Furnace Cavity - Hot Zone
Kgc	W/cm-°C	Conductivity of Gas in Furnace Cavity - Cold Zone
Ka	W/cm-°C	Conductivity of Ampoule
Ain	cm	Sample Radius
Ao	cm	Ampoule outer Radius
Afh	cm	Inside Radius of Furnace Muffle - Hot Zone
Afc	cm	Inside Radius of Furnace Muffle - Cold Zone
Ehot		Effective Emissivity of Ampoule/Sample - Hot Zone
Ecold		Effective Emissivity of Ampoule/Sample - Cold Zone
Efhot		Emissivity of Furnace Muffle - Hot Zone
Efcold		Emissivity of Furnace Muffle - Cold Zone
Lat	cm	Total Length of the Adiabatic Zone
Tla	°C	Sample Temperature at Edge of Adiabatic Zone - Hot Side
Tsa	°C	Sample Temperature at Edge of Adiabatic Zone - Cold Side
Lim	cm	$-Lim \leq X \leq Lim$ is range to Calculate Temperature Profiles. Must be an integer (plotter requirement).

TABLE A-3. SPECIFIC INPUT FOR CASE I

Variable	Units	Description
Rhos	g/cm^3	Average Sample Density
Rhoa	g/cm^3	Average Ampoule Density
Cps	W-sec/g-°C	Average Sample Specific Heat
Cpa	W-sec/g-°C	Average Ampoule Specific Heat
U	cm/sec	Ampoule Pull Rate
Dhf	W-sec/g	Heat of Fusion

TABLE A-4. SPECIFIC INPUT FOR CASE II

Variable	Units	Description
Bhstar		Biot Number at End of Sample - Hot Zone
Lc	cm	Length of the Ampoule Inserted into the Hot Zone

TABLE A-5. SPECIFIC INPUT FOR CASE III AND IV

Variable	Units	Description
Tb	°C	Temperature of Booster (Tickler) Heater
Lbt	cm	Length of the Booster (Tickler) Heater

TABLE A-6. SPECIFIC INPUT FOR CASE V

Variable	Units	Description
Tb	°C	Temperature of Booster (Tickler) Heater
Lbt	cm	Length of Booster (Tickler) Heater
Glt	- °C/cm	Gradient in Liquid at which to Optimize Adiabatic Zone Length. Note: Must be negative.

TABLE A-7. GENERAL INPUT FOR CASES I-V
(Reference Table A-2 for definitions and units)

Id$	Sample Case I (see Note 1)
Th	450
Tm	271.5
Tc	40
Kls	0.124
Kss	0.072
Hconvh	0 (see Note 2)
Hconvc	0.0312 (see Note 3)
Kgh	0.003
Kgc	0 (see Note 4)
Ka	0.02 (see Note 5)
Ain	0.5
Ao	0.6 (see Note 6)
Afh	2.6
Afc	1.77
Ehot	0.7695
Ecold	0.9486
Efhot	0.3
Efcold	0.3
Lat	2.03
Tla	327 (see Note 7)
Tsa	133 (see Note 8)
Lim	5 (see Note 9)

NOTES

1. I was replaced by II, III, IV, and V for the five cases respectively.
2. Heat transfer in the hot end was assumed to be dominated by conduction and radiation since the space between the sample and furnace muffle contained stagnant helium gas. A value of Hconvh = 0 was used here to model that assumption.
3. The convective heat transfer coefficient in the cold zone was estimated from the formula in the Thermal Model (page 15, Appendix B).
4. The conductive heat transfer of the gas was included in the empirical formula for forced convection, Thermal Model (page 15, Appendix B).
5. A fused silica ampoule was modeled and an average conductivity value used. Enter 0 here if no ampoule is included.

TABLE A-7. (Continued)

NOTES (Continued)

6. Enter Ao = Ain if no ampoule is used.
7. If this value is not known, a good first guess is Tla = (Th + Tm)/2. The interactive mode will allow for a correction, if necessary after the temperature profiles are calculated.
8. See note 7 and use Tsa = (Tc + Tm)/2 as the first guess.
9. Lim was set = 2 (integer required) in Case II because only 2.5 cm was inserted into the hot zone.

TABLE A-8. SPECIFIC INPUT FOR CASES I-V

Case I	Rhos = 10.05
	Rhoa = 2.3
	Cps = 0.1463
	Cpa = 0.493
	U = 0.0028
	Dhf = 50.16
Case II	Bhstar = 0.0507 (see Note 1)
	Lc = 2.5
Case III	T_b = 450 (see Note 2)
	Lbt = 0 (see Note 3)
Case IV	Tb = 450 (see Note 2)
	Lbt = 1.8 (see Note 3)
NOTE: An input for Tc = 40 was entered when general input was called for. This case will calculate a new value for Tc and run the temperature profiles with this new value.	
Case V	Tb = 500
	Lbt = 1.8
	Glt = -85 (see Note 4)

NOTES

1. Case III was run and the printed temperature profile was used to find T at x = Lc = -2.5. This T was then read in as input for Tla in Case III, and the calculated Biot number for the hot zone was used as Bhstar input for Case II.
2. If the booster heater is not used, this value should be set equal Th.
3. If the booster heater is not used (i.e., Tb = Th), Lbt may be any number ≥ 0.
4. This must be a negative number.

FLOW CHARTS

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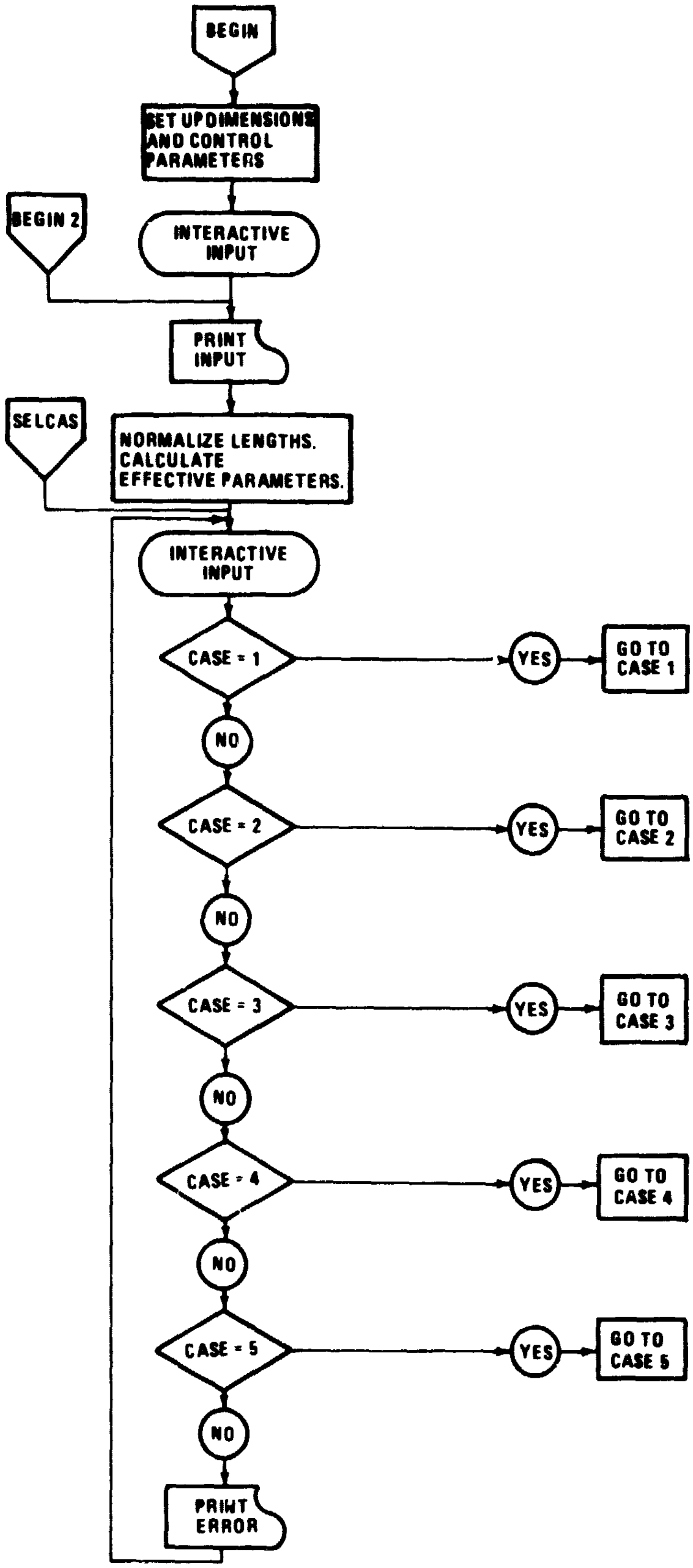
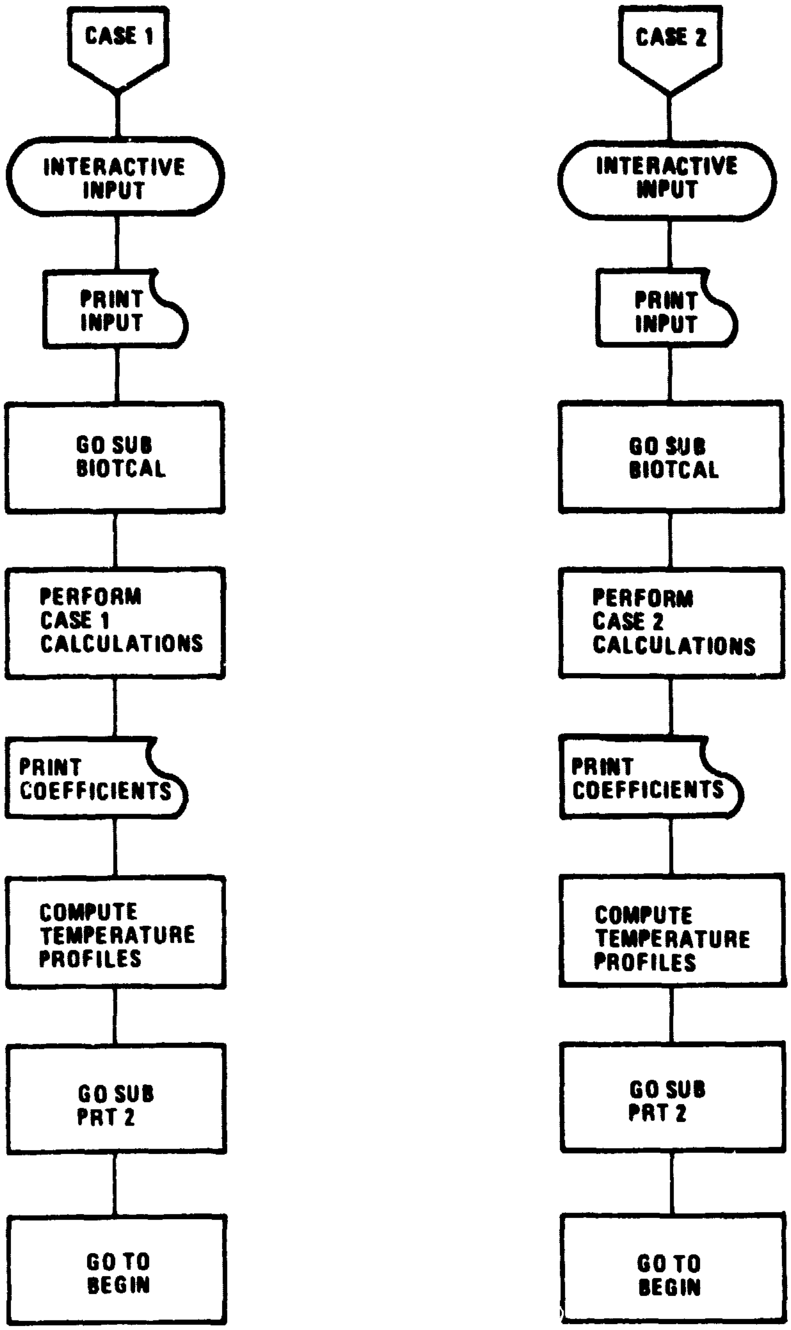
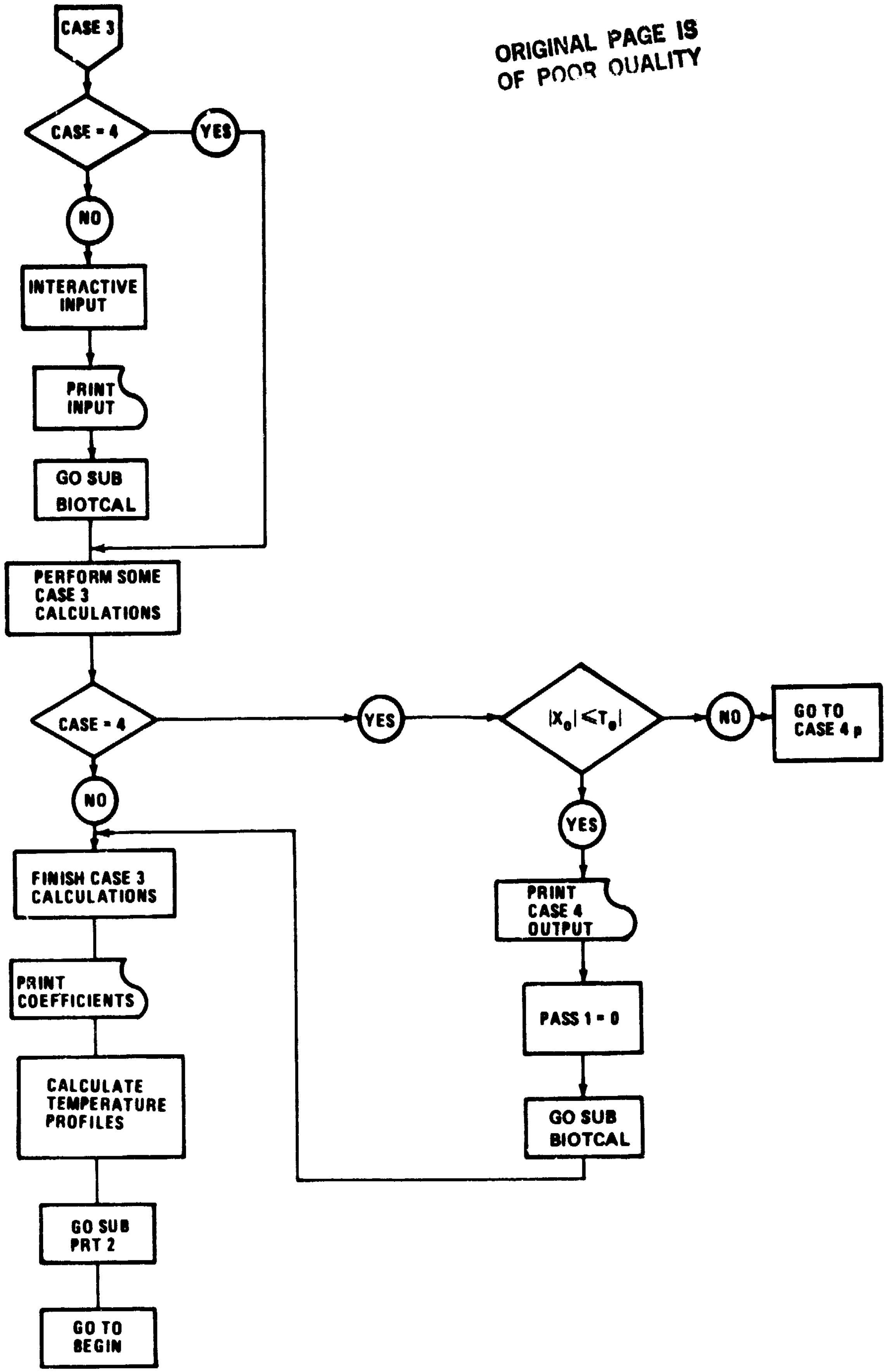



CASE 1
INTERACTIVE INPUT
PRINT INPUT
GO SUB BIOTCAL
PERFORM CASE 1 CALCULATIONS
PRINT COEFFICIENTS
COMPUTE TEMPERATURE PROFILES
GO SUB PRT 2
GO TO BEGIN
CASE 2
INTERACTIVE INPUT
PRINT INPUT
GO SUB BIOTCAL
PERFORM CASE 2 CALCULATIONS
PRINT COEFFICIENTS
COMPUTE TEMPERATURE PROFILES
GO SUB PRT 2
GO TO BEGIN


CASE 3
CASE = 4
YES
NO
INTERACTIVE INPUT
PRINT INPUT
GO SUB BIOTCAL
PERFORM SOME CASE 3 CALCULATIONS
CASE = 4
YES
$|X_e| \leq T_e|$
NO
GO TO CASE 4 p
NO
YES
FINISH CASE 3 CALCULATIONS
PRINT CASE 4 OUTPUT
PRINT COEFFICIENTS
PASS 1 = 0
CALCULATE TEMPERATURE PROFILES
GO SUB BIOTCAL
GO SUB PRT 2
GO TO BEGIN

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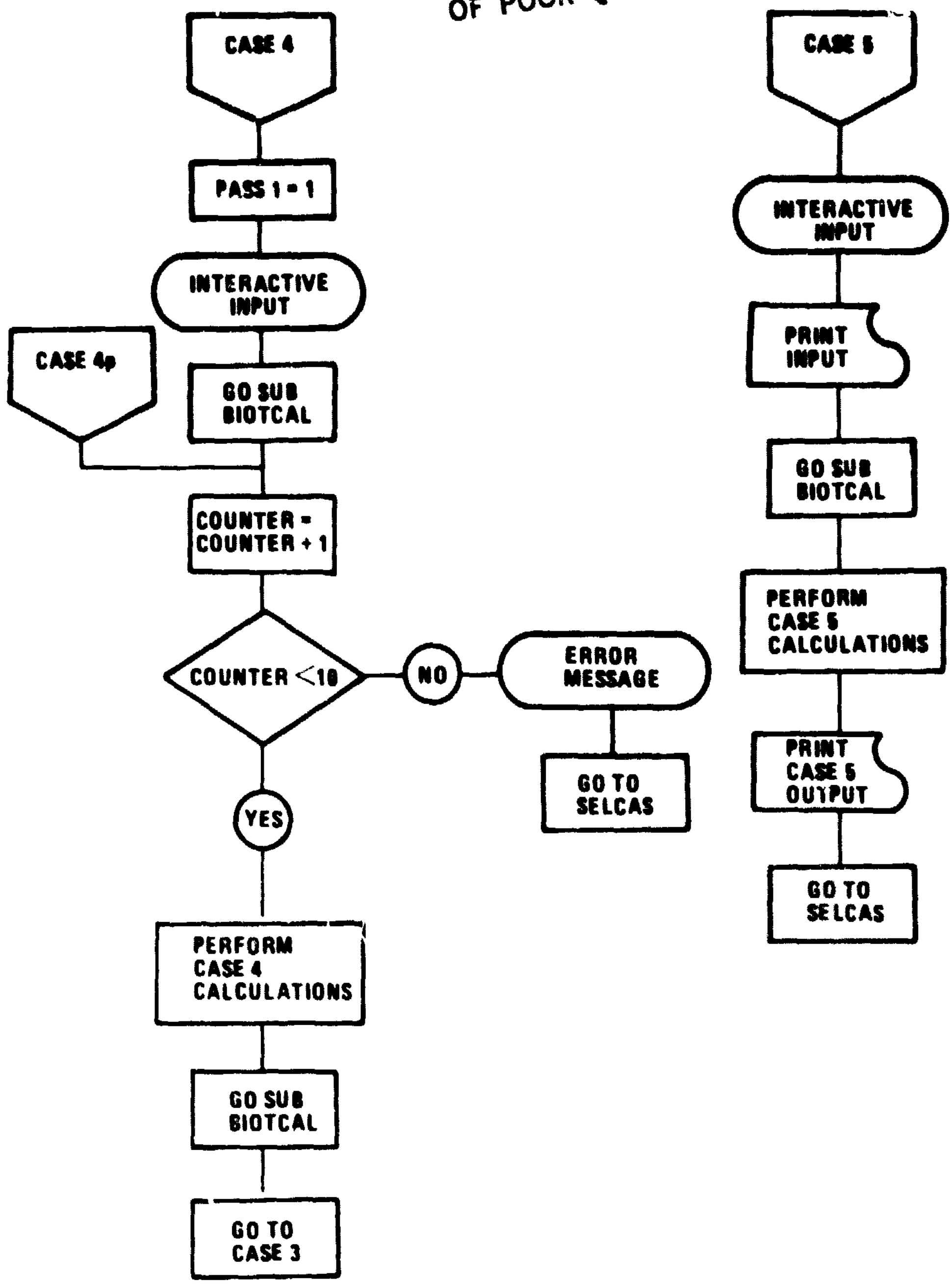
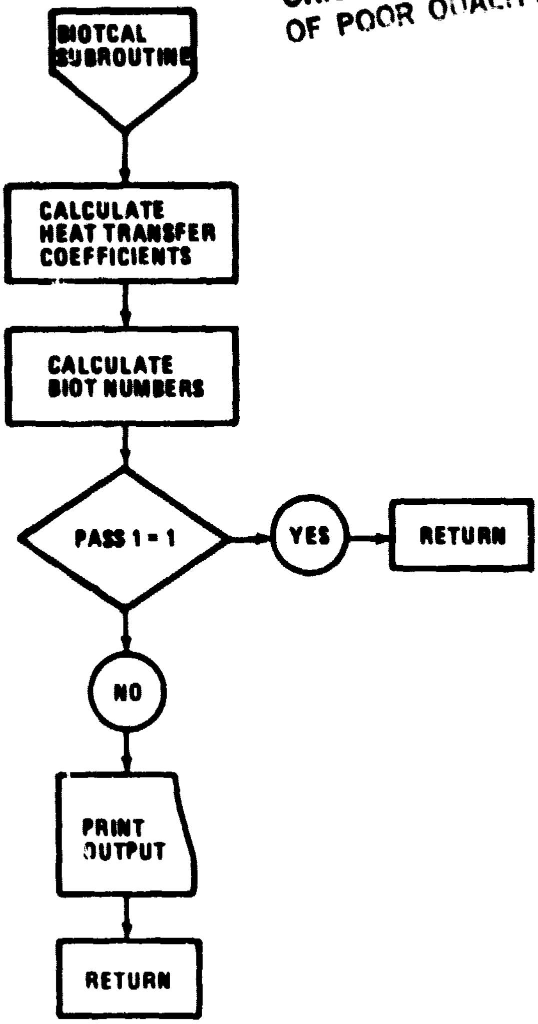
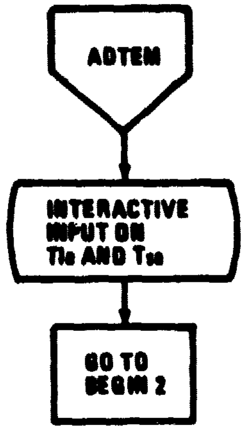
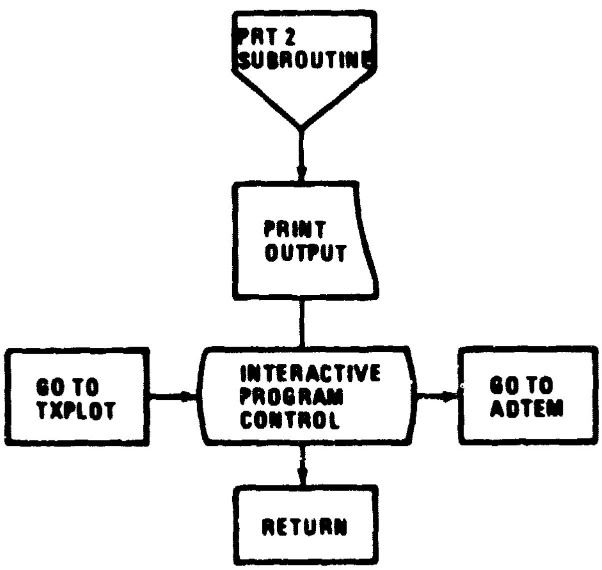
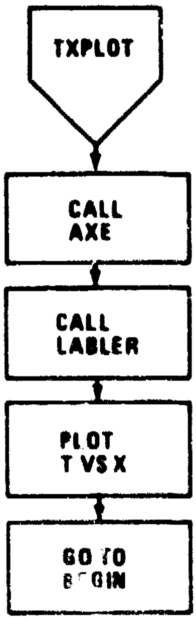
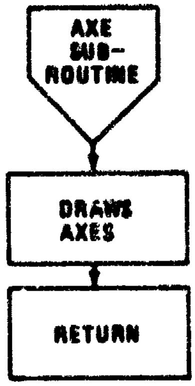


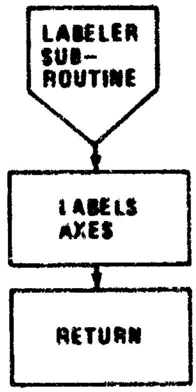

BIOTCAL SUBROUTINE
CALCULATE HEAT TRANSFER COEFFICIENTS
CALCULATE BIOT NUMBERS
PASS 1 = 1
YES
RETURN
NO
PRINT OUTPUT
RETURN


ADTEM
INTERACTIVE INPUT ON Tie AND Tse
GO TO BEGIN 2


PRT 2 SUBROUTINE
PRINT OUTPUT
GO TO TXPLOT
INTERACTIVE PROGRAM CONTROL
GO TO ADTEM
RETURN


TXPLOT
CALL AXE
CALL LABLER
PLOT T VS X
GO TO BEGIN


AXE SUB-ROUTINE
DRAWS AXES
RETURN


LABELER SUB-ROUTINE
LABELS AXES
RETURN

COMPUTER PROGRAM LISTING

```
10   '        AN ANALYTICAL APPROACH TO THERMAL MODELLING
20   '             OF BRIDGMAN-TYPE CRYSTAL GROWTH
30   '                ONE-DIMENSIONAL ANALYSIS
40   '
50   '        NEGATIVE X IS IN HOT ZONE OF FURNACE
60   '        X=0 IS IN MIDDLE OF ADIABATIC ZONE
70   '        POSITIVE X IS IN COLD ZONE OF FURNACE
80   '
90   DIM Xarray(101),Iarray(101)
100 Begin:  Counter=0  'ITERATION COUNTER
110  Case=0  'CASE SELECTION CONTROL
120  Pass1=0 'CASE4 CONTROL VARIABLE
130  INPUT " RUN IDENTIFICATION (18 CHARACTERS)",Id$
140  INPUT "TEMP. OF HOT ZONE ( DEG. C)",Th
150  INPUT "TEMP. OF MELT  INTERFACE (DEG. C)",Tm
160  INPUT "TEMP OF COLD ZONE (DEG. C)",Tc
170  INPUT "CONDUCTIVITY OF LIQUID (W/cm-C)",Kls
180  INPUT "CONDUCTIVITY OF SOLID (W/cm-C)",Kss
190  INPUT "CONVECTIVE HEAT TRANSFER COEFF. - HOT END (W/cm2-C)",Hconvh
200  INPUT "CONVECTIVE HEAT TRANSFER COEFF. -COLD END (W/cm2-C)",Hconvc
210  INPUT "CONDUCTIVITY OF GAS -HOT END- ( W/cm-C)",Kgh
220  INPUT "CONDUCTIVITY OF GAS -COLD END- (W/cm-C)",Kgc
230  INPUT "CONDUCTIVITY OF AMPOULE  ( W/cm-C)",Ka
240  INPUT "SAMPLE RADIUS  ( cm)",Ain
250  INPUT "AMPOULE OUTER RADIUS (cm)",Ao
260  INPUT "INSIDE RADIUS OF FURNACE MUFFLE IN HOT ZONE (cm)",Afh
270  INPUT "INSIDE RADIUS OF FURNACE MUFFLE IN THE COLD ZONE (cm)",Afc
280  INPUT "EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-HOT END-",Ehot
290  INPUT "EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-COLD END",Ecold
300  INPUT "EMISSIVITY OF FURNACE WALL -HOT END",Efhot
310  INPUT "EMISSIVITY OF FURNACE WALL -COLD END",Efcold
320  INPUT "LENGTH OF ADIABATIC ZONE (cm)",Lat
330  INPUT "TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE (DEG C)",Tla  'IF TEMP.
 IS NOT KNOWN-GUESS A VALUE,CHECK AFTER PROFILE IS CAL. AND CORRECT
340  INPUT "TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE (DEG C)",Tsa
350  INPUT "51 PT. TEMP. PROFILE WILL BE CAL. FOR -LIM<X<LIM. INPUT LIM(cm)",Lim
360 Begin2:     PRINTER IS 7,6  'PRINTER
370  PRINT
380  PRINT "                     1 D MODEL OF CRYSTAL GROWTH"
390  PRINT "                          ";Id$
400  PRINT
410  PRINT
420  PRINT "TEMPERATURE OF HOT ZONE (C)                              ",Th
430  PRINT "TEMPERATURE OF INTERFACE (C)                             ",Tm
440  PRINT "TEMPERATURE OF COLD ZONE (C)                             ",Tc
450  PRINT "CONDUCTIVITY OF LIQUID (W/cm-C)                          ",Kls
460  PRINT "CONDUCTIVITY OF SOLID (W/cm-C)                           ",Kss
470  PRINT "CONVECTIVE HEAT TRANSFER COEFF.-HOT END (W/cm2-C)",Hconvh
480  PRINT "CONVECTIVE HEAT TRANSFER COEFF.-COLD END(W/cm2-C)",Hconvc
490  PRINT "CONDUCTIVITY OF GAS - HOT END (W/cm-C)                   ",Kgh
500  PRINT "CONDUCTIVITY OF GAS - COLD END (W/cm-C)                  ",Kgc
510  PRINT "CONDUCTIVITY OF AMPOULE (W/cm-C)                         ",Ka
520  PRINT "SAMPLE RADIUS (cm)                                       ",Ain
530  PRINT "AMPOULE OUTER RADIUS (cm)                                ",Ao
540  PRINT "INSIDE RADIUS OF FURNACE MUFFLE IN HOT ZONE(cm)  ",Afh
550  PRINT "INSIDE RADIUS OF FURNACE MUFFLE IN COLD ZONE(cm) ",Afc
560  PRINT "EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-HOT END-  ",Ehot
570  PRINT "EFFECTIVE EMISSIVITY OF AMPOULE/SAMPLE-COLD END-",Ecold
580  PRINT "EMISSIVITY OF FURNACE -HOT END                           ",Efhot
590  PRINT "EMISSIVITY OF FURNACE  COLD END                          ",Efcold
600  PRINT "LENGTH OF ADIABATIC ZONE (cm)                            ",Lat
610  PRINT "TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE (C) ",Tla
620  PRINT "TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE (C)",Tsa
```

```
630  ! - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
640  !       NORMALIZE BY AO AND CALCULATE EFFECTIVE CONDUCTIVITIES
650  La=Lat/Ao
660  X1=La/2   !HALF LENGTH OF AD. ZONE
670  Xinc=2*Lim/50     !X INCREMENT FOR TEMP. PROFILES-SET FOR 51 POINTS
680  Xc=-Lim           !INITIAL X(cm) AT WHICH TO START TEMP. PROFILES
690  Kl=Kls*Ain^2/Ao^2+Ka*(1-Ain^2/Ao^2)     !EFFECTIVE CONDUCTIVITY-LIQUID
700  Ks=Kss*Ain^2/Ao^2+Ka*(1-Ain^2/Ao^2)    !EFFECTIVE CONDUCTIVITY-SOLID
710  PRINT "CALCULATED EFFECTIVE CONDUCTIVITY OF LIQUID (W/cm-C)",Kl
720  PRINT "CALCULATED EFFECTIVE CONDUCTIVITY OF SOLID (W/cm-C)  ",Ks
730  ! - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
740  !                          SELCAS
750  !                FOLLOWING ALLOWS VARIOUS CASE SELECTIONS
760  !
770 Selcas:     PRINTER IS 16    !CRT
780  PRINT "THE FOLLOWING RUN OPTIONS ARE AVAILABLE"
790  PRINT
800  PRINT "1. CASE I"
810  PRINT "2. CASE II"
820  PRINT "3. CASE III"
830  PRINT "4. CALCULATE (CASE III) OPTIMUM Tc TO CENTER THE MELT ISOTHERM"
840  PRINT "5. CALCULATE (CASE III) OPTIMUM La FOR A GIVEN GRADIENT"
850  PRINT
860  INPUT "INPUT 1,2,3,4, OR 5",Case
870  PRINTER IS 7,6   !PRINTER
880  IF Case=1 THEN Case1
890  IF Case=2 THEN Case2
900  IF Case=3 THEN Case3
910  IF Case=4 THEN Case4
920  IF Case=5 THEN Case5
930  PRINTER IS 16   !CRT
940  PRINT "ERROR IN LAST INPUT--RUN OPTION MUST =1,2,3,4,OR 5"
950  PRINT "PRESS: CONTINUE BAR FOR ANOTHER CHANCE TO INPUT RUN OPTION"
960  PAUSE
970  GOTO Selcas
980  !
990  !
1000 ! - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
1010 !                          BIOTCAL
1020 !     CALCULATES CONDUCTIVE AND RADIATIVE HEAT TRANSFER COEFF. AND BIOT NOS.
1030 !
1040 Biotcal: PRINTER IS 7,6   !PRINTER
1050 Feh=1/(1/Ehot+Ao/Afh*(1/Efhot-1))
1060 Fec=1/(1/Ecold+Ao/Afc*(1/Efcold-1))
1070 Hradh=5.67E-12*Feh*(25/12*(Th+273)^3+13/12*(Th+273)^2*(Tla+273)+7/12*(Th+27
3)*(Tla+273)^2+1/4*(Tla+273)^3)
1080 Hradc=5.67E-12*Fec*(25/12*(Tc+273)^3+13/12*(Tc+273)^2*(Tsa+273)+7/12*(Tc+27
3)*(Tsa+273)^2+1/4*(Tsa+273)^3)
1090 Hcondh=Kgh/Ao/LOG(Afh/Ao)
1100 Hcondc=Kgc/Ao/LOG(Afc/Ao)
1110 Hstarh=Hconvh+Hradh+Hcondh    !EFFECTIVE HEAT TRANSFER COEFF.-HOT END
1120 Hstarc=Hconvc+Hradc+Hcondc     !EFFECTIVE HEAT TRANSVER COEFF. - COLD END
1130 Bh=Hstarh*Ao/Kl          !BIOT NO. -HOT END
1140 Bc=Hstarc*Ao/Ks          !BIOT NO. -COLD END
1150 Alfa=SQR(2*Bc)
1160 Beta=SQR(2*Bh)
1170 IF Pass1=1 THEN RETURN     ! ALLOWS FOR TC ITERATION WITHOUT PRINT-CASE4
1180 PRINT
1190 PRINT
1200 PRINT "CALCULATED EMISSIVITY FUNCTION (Feh)-HOT            ",Feh
1210 PRINT "CALCULATED EMISSIVITY FUNCTION (Fec)-COLD           ",Fec
1220 PRINT "CALCULATED RADIATIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)",Hradh
1230 PRINT "CALCULATED RADIATIVE HEAT TRANS. COEFF.-COLD (W/Cm2-C)",Hradc
```

```
1240 PRINT "CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-HOT (W/cm2-C)",Hcondh
1250 PRINT "CALCULATED CONDUCTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)",Hcondc
1260 PRINT "CALCULATED EFFECTIVE HEAT TRANS. COEFF.-HOT(W/cm2-C)  ",Hstarh
1270 PRINT "CALCULATED EFFECTIVE HEAT TRANS. COEFF.-COLD(W/cm2-C)  ",Hstarc
1280 PRINT "CALCULATED BIOT NO. -HOT END-                          ",Bh
1290 PRINT "CALCULATED BIOT NO. -COLD END-                         ",Bc
1300 RETURN
1310 '
1320 ' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
1330 !
1340 '                        CASE I
1350 ' FOLLOWING CALCULATES TEMP. PROFILES IN A SAMPLE AS IT IS BEING TRANSLATED
1360 '      AT A VELOCITY U
1370 '
1380 Case1:    PRINT
1390 PRINT
1400 PRINT "                        CASE 1"
1410 PRINT
1420 PRINT
1430 INPUT "AVERAGE SAMPLE DENSITY (g/cm3)",Rhos
1440 INPUT "AVERAGE AMPOULE DENSITY (g/cm3)",Rhoa
1450 INPUT "AVERAGE SAMPLE SPECIFIC HEAT (W-sec/g-C)",Cps
1460 INPUT "AVERAGE AMPOULE SPECIFIC HEAT (W-sec/g-C)",Cpa
1470 INPUT "AMPOULE VELOCITY (cm/sec)",U
1480 INPUT "HEAT OF FUSION (W-sec/g)",Dhf
1490 PRINT "AVERAGE SAMPLE DENSITY (g/cm3)                  ",Rhos
1500 PRINT "AVERAGE AMPOULE DENSITY (g/cm3)                 ",Rhoa
1510 PRINT "AVERAGE SAMPLE SPECIFIC HEAT (W-sec/g-C)         ",Cps
1520 PRINT "AVERAGE AMPOULE SPECIFIC HEAT (W-sec/g-C)       ",Cpa
1530 PRINT "AMPOULE VELOCITY (Cm/sec)                        ",U
1540 PRINT "HEAT OF FUSION (W-sec/g)                         ",Dhf
1550 Rceff=Rhos*Cps*Ain^2/Ao^2+Rhoa*Cpa*(1-Ain^2/Ao^2)
1560 Dhfeff=Dhf*Ain^2/Ao^2
1570 Rhoeff=Rhos*Ain^2/Ao^2+Rhoa*(1-Ain^2/Ao^2)
1580 Pl=Rceff*Ao*U/Kl
1590 Ps=Kl*Pl/Ks
1600 PRINT "CALCULATED PECLEC NO. FOR THE LIQUID             ",Pl
1610 PRINT "CALCULATED PECLEC NO. FOR THE SOLID              ",Ps
1620 GOSUB Biotcal
1630 Lf=Rhoeff*Ao*U*Dhfeff
1640 Astar=(SQR(4*Alfa^2+Ps^2)-Ps)/2
1650 Bstar=(SQR(4*Beta^2+Pl^2)+Pl)/2
1660 Lam1=(Ps*Kl*(Th-Tm)*(X1^2/2+X1/Astar)+Pl*Ks*(Tm-Tc)*(X1^2/2+X1/Bstar)+Lf*(X
1-1/Astar)*(X1*1/Bstar))/(Kl*(Th-Tm)+Ks*(Tm-Tc))
1670 Lam2=Lf*(1/Bstar-1/Astar)+Ps*Ks*(Tm-Tc)*(X1+1/Bstar)-Pl*Kl*(Th-Tm)*(X1+1/As
tar)
1680 Lam2=Lam2/(Kl*(Th-Tm)+Ks*(Tm-Tc))
1690 Lam3=(Lf+Ps*(Kl*(Th-Tm)/2+Ks*(Tm-Tc))+Pl*(Ks*(Tm-Tc)/2+Kl*(Th-Tm)))/(Kl*(Th
-Tm)+Ks*(Tm-Tc))
1700 Dx0=Lam1-Lam2*X0-Lam3*X0^2
1710 X0p=X0+Dx0
1720 GOSUB Residue
1730 ' - -  - - - - - - - - -
1740 Res1=Res
1750 X0p=X0p+.01
1760 GOSUB Residue
1770 Res2=Res
1780 X0=X0p+.01*Res2/(Res1-Res2)
1790 IF ABS(Res1)<.00001 THEN Pop !TEST  FOR CONVERGENCE
1800 X0p=X0
1810 GOSUB Residue
1820 GOTO 1740
1830 '    - - - - - - - - - - - -
```

```
1840 Residue:Lres=K1*P1*(Tm-Th)*EXP(P1*X0p)/(EXP(-P1*X1)*(P1/Bstar-1)+EXP(P1*X0p
))-L1
1850 Rres=Ks*Ps*(Tc-Tm)*EXP(Ps*X0p)/(EXP(Ps*X1)*(Ps/Astar+1)-EXP(Ps*X0p))
1860 Res=Rres-Lres
1870 RETURN
1880 ! --- - - - - - - - - - - - - -
1890 Pop:           ! X0 HAS CONVERGED
1900 B=(Tm-Th)/(EXP(-P1*X1)*(P1/Bstar-1)+EXP(P1*X0))
1910 Bprime=(Tc-Tm)/(EXP(Ps*X1)*(Ps/Astar+1)-EXP(Ps*X0))
1920 A=B*EXP(-P1*X1)*(P1/Bstar-1)+Th
1930 Aprime=-Bprime*EXP(Ps*X1)*(Ps/Astar+1)+Tc
1940 C=-Ps*Bprime*EXP(Ps*X1)/Astar
1950 D=-P1*B*EXP(-P1*X1)/Bstar
1960 G1=P1*B*EXP(P1*X0)
1970 Gs=Ps*Bprime*EXP(Ps*X0)
1980 PRINT
1990 PRINT "THE FOLLOWING COEFFICIENTS ARE USED IN CALCULATING TEMPERATURE"
2000 PRINT "A=";A;"B=";B;"ASTAR=";Aprime;"BSTAR=";Bprime;"C=";C;"D=";D
2010 FOR I=1 TO 51    ! CALCULATE 51 PT. TEMP. PROFILE
2020 X=Xc/Ao   !NORMALIZE
2030 IF X<-X1 THEN T=Th-D*EXP(Bstar*(X+X1))
2040 IF (X>-X1) AND (X<X0) THEN T=A+B*EXP(P1*X)
2050 IF (X>X0) AND (X<X1) THEN T=Aprime+Bprime*EXP(Ps*X)
2060 IF X>X1 THEN T=Tc+C*EXP(-Astar*(X-X1))
2070 Xarray(I)=Xc
2080 Tarray(I)=T
2090 Xc=Xc+Xinc
2100 NEXT I
2110 GOSUB Prt2   !PRINT OUTPUT
2120 GOTO Begin   !PROGRAM SHOULD NORMALLY NEVER EXECUTE THIS
2130 !
2140 ! - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
2150 !                         CASE II
2160 ! INVESTIGATION OF END EFFECTS-SAMPLE IS INSERTED A FINITE DISTANCE LC IN
2170 !      THE HOT ZONE.  SAMPLE IS MOTIONLESS.
2180 !
2190 Case2:  PRINT
2200 PRINT "                        CASE II"
2210 PRINT
2220 PRINT
2230 INPUT "BIOT NO. (B*) AT END OF ROD IN THE HOT ZONE     ",Bhstar
2240 INPUT "LENGTH OF THE  AMPOULE WHICH IS  INSERTED INTO HOT ZONE (cm)",Lc
2250 PRINT "BIOT NO. AT END OF ROD IN HOT ZONE              ",Bhstar
2260 PRINT "LENGTH OF AMPOULE INSERTED INTO HOT ZONE (cm)   ",Lc
2270 GOSUB Biotcal
2280 L=Lc/Ao   !NORMALIZE
2290 F1=((1+Bhstar/Beta)*EXP(Beta*L)+(1-Bhstar/Beta)*EXP(-Beta*L))/((1+Bhstar/Be
ta)*EXP(Beta*L)-(1-Bhstar/Beta)*EXP(-Beta*L))
2300 G1=-(Th-Tm+Ks/K1*(Tm-Tc))/(La+1/Alfa+F1/Beta)
2310 Gs=K1*G1/Ks
2320 X0=(K1*(Th-Tm)*(X1+1/Alfa)-Ks*(Tm-Tc)*(X1+F1/Beta))/(K1*(Th-Tm)+Ks*(Tm-Tc))
2330 T0=Tm-G1*X0
2340 T0star=Tm-Gs*X0
2350 C=-Gs/Alfa
2360 B=G1*EXP(-Beta*L)/Beta/((1+Bhstar/Beta)/(1-Bhstar/Beta)*EXP(Beta*(L+La))-EX
P(-Beta*(L-La)))
2370 D=-G1/Beta/(1-(1-Bhstar/Beta)/(1+Bhstar/Beta)*EXP(-2*Beta*L))
2380 PRINT
2390 PRINT "THE FOLLOWING COEFFICIENTS ARE USED IN CALCULATING TEMPERATURE"
2400 PRINT "B=";B;"C=";C;"D=";D
2410 FOR I=1 TO 51     !CAL. 51 PT. TEMP. PROFILE
2420 X=Xc/Ao   !NORMALIZE
2430 IF X<-X1 THEN T=Th-D*EXP(Beta*(X+X1))+B*EXP(-Beta*(X-X1))
```

```
2440 IF (X>-X1) AND (X<X0) THEN T=T0+G1*X
2450 IF (X>X0) AND (X<X1) THEN T=TGstar+Gs*X
2460 IF X>X1 THEN T=Tc+C*EXP(-Alfa*(X-X1))
2470 Xarray(I)=Xc
2480 Tarray(I)=T
2490 Xc=Xc+Xinc
2500 NEXT I
2510 GOSUB Prt2  !PRINT OUTPUT
2520 GOTO Begin  !PROG. WILL NOT NORMALLY  EXECUTE THIS STEP
2530 !
2540 !
2550 ! - - - - - - - - - - - - - - - - - - - - - - - - - - - -- - - - - - - - -
2560 !                              CASE III
2570 ! STEADY STATE CALCULATION WITH AN OPTIONAL TICKLER HEATER
2580 !
2590 Case=3:  IF Case=4 THEN GOTO 2700        !INPUT HAS ALREADY BEEN SUBMITTED
2600 X1=La/2    ! 1/2 OF AD. ZONE LENGTH
2610 PRINT
2620 PRINT "                         CASE III"
2630 PRINT
2640 INPUT "TEMP. OF TICKLER HEATER (DEG. C)",Tb
2650 INPUT "LENGTH OF TICKLER HEATER (cm)    ",Lbt
2660 PRINT "TEMPERATURE OF TICKLER HEATER (C)                  ",Tb
2670 PRINT "LENGTH OF TICKLER HEATER (cm)                      ",Lbt
2680 GOSUB Biotcal
2690 !     CALCULATES GRADIENT AND X0 POSITION FROM CENTER LINE
2700 Lb=Lbt/Ao           !NORMALIZE LENGTH TO AMPOULE OUTER RADIUS
2710 Lb2=Lb/2
2720 X2=X1+Lb2
2730 X3=X2+Lb2
2740 Ealfa=EXP(Alfa*Lb2)
2750 Ebeta=EXP(Beta*Lb2)
2760 B=-(Tb-Th)/2/Ebeta
2770 G1=-(Tb-Tm+Ks/K1*(Tm-Tc)+(Th-Tb)*EXP(-Beta*Lb))/(La+1/Beta+1/Alfa)
2780 X0=-(Tb-Tm+(Th-Tb)*EXP(-Beta*2*Lb2)-Ks/K1*(Tm-Tc)+G1*(1/Beta-1/Alfa))/2/G1
2790 IF Case<>4 THEN GOTO Case3p   !SKIP FOLLOWING TEST IF NOT IN CASE4
2800 IF ABS(X0)>1E-6 THEN GOTO Case4p  !ALLOWS FOR TC ITERATION
2810 !
2820 ! X0 IS WITHIN TOLERANCE FOR CENTER OF AD. ZONE ON CASE 4
2830 PRINT "CALCULATED Tc(C)                                   ",Tc
2840 PRINT "TEMPERATURE OF TICKLER HEATER (C)                   ",Tb
2850 PRINT "LENGTH OF TICKLER HEATER (cm)                       ",Lbt
2860 Pass1=0    !RESET CASE TO ALLOW FOR PRINT IN BIOTCAL
2870 GOSUB Biotcal
2880 !
2890 Case3p: Gs=K1*G1/Ks
2900 C=-Gs/Alfa
2910 A=(B/Ebeta+G1/Beta)/Ebeta
2920 D=-A/Ebeta+B*Ebeta
2930 T0=Tm-G1*X0
2940 T0s=Tm-Gs*X0
2950 PRINT
2960 PRINT "THE FOLLOWING COEFFICIENTS ARE USED IN CALCULATING TEMPERATURE"
2970 PRINT "A=";A;"B=";B;"C=";C;"D=";D
2980 FOR I=1 TO 51
2990 X=Xc/Ao   !CAL. 51 PT. TEMP. PROFILE
3000 IF X<=-X3 THEN T=Th-D*EXP(Beta*(X+X3))
3010 IF (X>-X3) AND (X<=-X1) THEN T=Tb+A*EXP(Beta*(X+X2))+B*EXP(-Beta*(X+X2))
3020 IF (X>-X1) AND (X<=X0) THEN T=T0+G1*X
3030 IF (X>X0) AND (X<=X1) THEN T=T0s+Gs*X
3040 IF X>X1 THEN T=Tc+C*EXP(-Alfa*(X-X1))
3050 Xarray(I)=Xc
3060 Tarray(I)=T
```

```
3070 Xc=Xc+Xinc
3080 NEXT I
3090 GOSUB Prt2
3100 GOTO Begin  !PROGRAM WILL NOT NORMALLY EXECUTE THIS STEP
3110 ! - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
3120 !                          CASE IV
3130 !    CALCULATES Tc WHICH WILL CENTER THE Tmelt ISOTHERM
3140 !        TEMPERATURE CALCULATIONS USES CASE III EQ.
3150 !
3160 Case4:  PRINT
3170 PRINT
3180 PRINT "                CASE IV     Tc CALCULATION"
3190 PRINT
3200 Pass1=1   ! CONTROL FOR FIRST PASS IN BIOTCAL
3210 INPUT "TEMP. OF TICKLER HEATER (Deg C)",Tb
3220 INPUT "LENGTH OF TICKLER HEATER (cm)",Lbt
3230 GOSUB Biotcal
3240 Lb=Lbt/Ao    !NORMALIZE
3250 Case4p:  ! ENTER CASE4 FOR ITERATION LOOP
3260 Counter=Counter+1    !ITERATION COUNTER
3270 IF Counter<10 THEN GOTO Case4pp
3280 PRINT "   Tc TO CENTER Tm ISOTHERM IN MIDDLE OF AD. ZONE WAS NOT FOUND AFTE
R 10 TRYS"
3290 PRINT "Tc=",Tc,"X0=",X0
3300 GOTO Selcas
3310 !
3320 Case4pp:
3330 Tc=Tm*(La+1/Beta+1/Alfa)/(La/2+1/Beta)-Kl/Ks*(La/2+1/Alfa)*(Tb-Tm+(Th-Tb)*E
XP(-Beta*Lb)+Ks/Kl*Tm)/(La/2+1/Beta)
3340 GOSUB Biotcal   !RECALCULATE ALFA AND BETA FOR NEXT ITERATION
3350 GOTO Case3
3360 ! - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
3370 !
3380 !                          CASE V
3390 !      CALCULATES OPTIMUM LENGTH OF ADIABATIC ZONE (LA)  TO ACHIEVE
3400 !          DESIGNATED LIQUID GRADIENT
3410 !
3420 Case5:  PRINT
3430 PRINT
3440 PRINT "      CASE V        CALCULATES OPTIMUM La FOR GIVEN GRADIENT"
3450 PRINT
3460 INPUT "TEMP. OF TICKLER HEATER (Deg C)",Tb
3470 INPUT "LENGTH OF TICKLER HEATER (cm)",Lbt
3480 INPUT "GRADIENT IN LIQUID (MINUS C/Cm) AT WHICH TO OPTIMIZE AD. ZONE LENGTH
",Glt
3490 PRINT "TEMPERATURE OF TICKLER HEATER (C)                ",Tb
3500 PRINT "LENGTH OF TICKLER HEATER (cm)                    ",Lbt
3510 Lb=Lbt/Ao !NORMALIZE
3520 Gl=Glt*Ao  !NORMALIZE
3530 GOSUB Biotcal
3540 La=(-Tb+Tm+(Tb-Th)*EXP(-Beta*Lb)-Ks/Kl*(Tm-Tc)-Gl*(1/Alfa+1/Beta))/Gl
3550 PRINT
3560 PRINT
3570 PRINT "FOR LIQUID GRADIENT =";Glt;"(C/cm)  AD. ZONE LENGTH=";La*Ao;"(cm)"
3580 PRINT
3590 PRINT "NOTE:    IF AD. ZONE LENGTH IS NEGATIVE--INPUT GRADIENT CANNOT BE AC
HIEVED WITH"
3600 PRINT "         GIVEN PARAMETERS."
3610 PRINT
3620 PRINT
3630 PRINT "NOTE:     THE AD. ZONE LENGTH HAS BEEN CHANGED IN PROG.  RUN CASE II
I FOR TEMP."
3640 PRINT "          PROFILES"
```

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3650 GOTO Selcms
3660 ! - - - - - - - - - - - - - - - - - - - - -
3670 !                              PRT2
3680 Prt2:      ! OUTPUT AND PROGRAM CONTROL
3690 PRINT
3700 PRINT
3710 PRINT "INTERFACE POSITION Xo (cm)               ",X0*Ao
3720 PRINT "GRADIENT IN LIQUID AT Xo  (deg C/cm)       ",Gl/Ao
3730 PRINT "GRADIENT IN SOLID AT Xo   (deg C/cm)       ",Gs/Ao
3740 PRINT
3750 PRINT
3760 PRINT "     TEMPERATURE PROFILE"
3770 PRINT "    X(cm)              T(C)"
3780 FOR I=1 TO 51    !PRINT 51 PT. TEMP. PROFILE
3790 PRINT Xarray(I),Tarray(I)
3800 NEXT I
3810 PRINTER IS 16  !CRT
3820 PRINT "    " !CLEAR CRT SCREEN
3830 PRINT "CHECK TEMP. AT HOT AND COLD EDGE OF ADIABATIC ZONE (X=+-1/2La)"
3840 PRINT "1. IF TEMP. ARE O.K.  TYPE:  CONT TXPLOT"
3850 PRINT "                             PRESS: EXECUTE KEY"
3860 PRINT "2. IF TEMP. NEED CORRECTING    TYPE:  CONT ADTEM "
3870 PRINT "                                     PRESS: EXECUTE KEY"
3880 PAUSE !SEE ABOVE INSTRUCTIONS TO CONTINUE PROGRAM
3890 RETURN
3900 ! - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
3910 !       ALLOWS ONE TO CORRECT INPUT TLA AND TSA TEMPERATURES
3920 Adtem:  INPUT "TEMP. OF SAMPLE AT HOT END OF ADIABATIC ZONE(C)",Tlm
3930 INPUT "TEMP. OF SAMPLE AT COLD END OF ADIABATIC ZONE(C)",Tsm
3940 GOTO 360
3950 ! - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
3960 !                          TXPLOT
3970 !            PLOTS X vs T FOR -Lim < X < Lim
3980 !
3990 Txplot:  PLOTTER IS 7,5,"9872A"
4000 DIM Titlet$(3)
4010 Titlet$(1)=Id$     !SET PLOT ID. EQUAL TO PROGRAM ID.
4020 ! INPUT "MAIN TITLE FOR X vs T PLOT --18 CHARACTERS",Titlet$(1)
4030 Titlet$(2)="X(cm)    "
4040 Titlet$(3)="TEMP(C)"
4050 LIMIT 0,190,0,190
4060 CALL Axe(-Lim,Lim,0,Th,1,50,-Lim,0,1) !IF LIM IS NOT AN INTEGER, AXE WILL A
SSUME THE NEXT LARGER INTERGER
4070 CALL Labler(-Lim,Lim,0,Th,-Lim,0,Titlet$(*))
4080 MOVE -Lim,Th
4090 FOR I=1 TO 51
4100 DRAW Xarray(I),Tarray(I)  !DRAW X vs T    !PLOT 51 PT. TEMP. PROFILE
4110 NEXT I
4120 !           DRAW Tmelt LINE
4130 MOVE -Lim,Tm
4140 DRAW Lim,Tm
4150 !           DRAW LEFT SIDE OF ADIABATIC ZONE
4160 Left=-Lat/2
4170 MOVE Left,0
4180 DRAW Left,Th
4190 !           DRAW MIDDLE OF ADIABATIC ZONE
4200 MOVE 0,0
4210 DRAW 0,Th
4220 !           DRAW RIGHT SIDE OF ADIABATIC ZONE
4230 MOVE -Left,0
4240 DRAW -Left,Th
4250 GOTO Begin      !START ALL OVER
4260 !
```

```
4270 ! - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - --
4280 !                          AXE
4290 !                  SCALES AND DRAWS AXES
4300 !
4310    SUB Axe(Xmin,Xmax,Ymin,Ymax,Xint,Yint,Xorg,Yorg,Type)      !--- Axe
        Rev. A
4320    DEF FNLow=(Yorg-Ymin<=.67*Height)
4330    DEF FNLeft=(Xorg-Xmin<=.67*Width)
4340    CSIZE 2.5,.5
4350    Height=Ymax-Ymin
4360    Width=Xmax-Xmin
4370    SCALE Xmin-ABS((.001+.1*FNLeft)*Width),Xmax+ABS((.05+.1*NOT FNLeft)*Width
),Ymin-ABS((.1+.12*FNLow)*Height),Ymax+ABS((.1+.12*NOT FNLow)*Height)
4380    CLIP Xmin,Xmax,Ymin,Ymax
4390    AXES Xint,Yint,Xorg,Yorg
4400    DEG
4410    LDIR 0
4420    LORG 2
4430      IF FNLeft THEN LORG 8
4440    Power=INT(LGT(Yint))
4450    Logscl=INT((Type-1)/2)
4460    Sign=1
4470    Yend=Ymax
4480    FOR I=1 TO 2
4490        FOR Yy=Yorg TO Yend STEP Sign*ABS(Yint)
4500            IF (Sign=-1) AND (Yy=Yorg) THEN Nxty
4510               MOVE Xorg,Yy
4520                 IF (Yy=Yorg) AND (Xmin<>Xorg) AND (Xmax<>Xorg) THEN MOVE Xor
g,Yy+(FNLow-NOT FNLow)*.02*Height
4530               Lab=Yy
4540                 IF Logscl THEN Lab=DROUND(10^Yy,3)
4550               GOSUB Label
4560                 IF FNLeft THEN LABEL USING "#,"&Fmt$&",X";Lab
4570                 IF NOT FNLeft THEN LABEL USING "#,X,"&Fmt$;Lab
4580 Nxty: NEXT Yy
4590        Sign=-1
4600        Yend=Ymin
4610    NEXT I
4620    LDIR 90
4630    LORG 2
4640      IF FNLow THEN LORG 8
4650    Power=INT(LGT(Xint))
4660    Logscl=NOT (Type MOD 2)
4670    Sign=1
4680    Xend=Xmax
4690    FOR I=1 TO 2
4700        FOR Xx=Xorg TO Xend STEP Sign*ABS(Xint)
4710            IF (Sign=-1) AND (Xx=Xorg) THEN Nxtx
4720               MOVE Xx,Yorg
4730                 IF (Xx=Xorg) AND (Ymin<>Yorg) AND (Ymax<>Yorg) THEN PLOT Xx+
(FNLeft-NOT FNLeft)*.02*Width,Yorg
4740               Lab=Xx
4750                 IF Logscl THEN Lab=DROUND(10^Xx,3)
4760               GOSUB Label
4770                 IF FNLow THEN LABEL USING "#,"&Fmt$&",X";Lab
4780                 IF NOT FNLow THEN LABEL USING "#,X,"&Fmt$;Lab
4790 Nxtx: NEXT Xx
4800        Sign=-1
4810        Xend=Xmin
4820    NEXT I
4830    GOTO Done
4840 Label: IF (ABS(Lab)>=100000) OR (ABS(Lab)<.001) OR (Power<=-6) AND (Lab<>0)
 THEN Fmt$="MD.DE"
```

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4850          IF Lab=0 THEN Fmt$="MD"
4860        IF (ABS(Lab))=100000) OR (ABS(Lab)<.001) OR (Power<=-6) OR (Lab=0) THE
N Ret
4870           Dig=INT(LGT(ABS(Lab)))
4880             IF Logscl AND (Dig<0) THEN Fmt$="M."&VAL$(ABS(Dig)+1)&"D"
4890             IF Dig>=0 THEN Fmt$="M"&VAL$(Dig+1)&"D"
4900           IF Logscl THEN Ret
4910              IF (Dig<0) AND (Dig>Power) THEN Fmt$="M."&VAL$(ABS(Power)+1)&"D"
4920              IF (Dig<0) AND (Dig<=Power) THEN Fmt$="M."&VAL$((ABS(Dig)+1)*(Di
g>-6)+6*(Dig<=-6))&"D"
4930              IF (Power<0) AND (ABS(Power)<6-Dig) AND (Dig>=0) THEN Fmt$=Fmt$&
"."&VAL$(ABS(Power)+1)&"D"
4940              IF (Power<0) AND (ABS(Power))=6-Dig) AND (Dig>=0) THEN Fmt$=Fmt$
&"."&VAL$(6-Dig)&"D"
4950 Ret: RETURN
4960 Done: SUBEND
4970    SUB Labler(Xmin,Xmax,Ymin,Ymax,Xorg,Yorg,Title$(*))       !--- Labler
        Rev. A
4980    DEF FNLow=(Yorg-Ymin<=.67*Height)
4990    DEF FNLeft=(Xorg-Xmin<=.67*Width)
5000    Height=ABS(Ymax-Ymin)
5010    Width=ABS(Xmax-Xmin)
5020    LDIR 0
5030    LORG 6
5040      IF FNLow THEN LORG 4
5050    MOVE Xmin+Width/2,FNLow*(Ymax+.07*Height)+NOT FNLow*(Ymin-.07*Height)
5060    LABEL USING "#,K";Title$(1)
5070    LORG 4
5080      IF FNLow THEN LORG 6
5090    MOVE FNLeft*Xmax+NOT FNLeft*Xmin,Yorg+FNLow*(.05*Height)-NOT FNLow*(.05*H
eight)
5100    LABEL USING "#,K";Title$(2)
5110    LORG 4
5120      IF FNLow THEN LORG 6
5130    MOVE Xorg,FNLow*(Ymax+.05*Height)+NOT FNLow*(Ymin-.05*Height)
5140    LABEL USING "#,K";Title$(3)
5150    SUBEND
```

APPENDIX B

AN ANALYTICAL APPROACH TO THERMAL MODELING OF BRIDGMAN-TYPE CRYSTAL GROWTH: ONE-DIMENSIONAL ANALYSIS

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AN ANALYTICAL APPROACH TO THERMAL MODELING OF BRIDGMAN-TYPE CRYSTAL GROWTH

I. ONE-DIMENSIONAL ANALYSIS

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ABSTRACT

The analysis of heat flow in directional solidification and crystal growth by Bridgman-type processes has received considerable attention in recent years. Since the problem is complex, particularly when detailed descriptions of furnace and sample properties are included, numerical techniques are often employed. While such techniques are indispensable for modeling of real systems, it is valuable to have available analytical methods, albeit simplified, to check and to guide the numerical analysis, to perform sensitivity analyses, and to perform trade studies on furnace design.

This work develops a one-dimensional analvtical description of the heat flow in a translating rod that is applicable for Biot numbers less than unity. The model can accommodate different properties of the sample in the solid and molten state, different heat transfer coefficients in the hot and cold zone, finite length effects in one zone, and approximates ampoule effects by adjusting the Biot numbers to account for heat transfer in the ampoule. Also, the model contains an adiabatic zone and a booster heater zone that can be used to increase the thermal gradient near the solidification interface or to provide an independent control over the position of the interface. Trade studies are performed on optimizing the length of the booster heater zone to obtain the maximum gradient in the sample without exceeding a specified maximum sample temperature.

AN ANALYTICAL APPROACH TO THERMAL MODELING OF BRIDGMAN-TYPE CRYSTAL GROWTH

I. ONE-DIMENSIONAL ANALYSIS

INTRODUCTION

In the design of vertical Bridgman-type directional solidification experiments, it is important to be able to predict the thermal profiles in the specimen. Of particular interest to the control of the process are the position and shape of the solidification interface and the axial thermal gradients on each side of the interface. Generally, this problem requires the use of numerical methods to obtain the required solutions. While such techniques are necessary to take into account the details of real systems, the insight and ability to determine how variations in the controllable parameters affect the conditions near the interface are diminished. For this purpose, it is desirable to have an approximate analytical solution to guide the numerical modeling and the experimental procedures.

Chang and Wilcox [1] solved the two-dimensional heat flow equation for a translating infinite cylinder with uniform physical properties in a two-zone furnace. Equal heat transfer coefficients in the hot and cold zone were assumed in order to obtain an analytical solution. A one-dimensional analysis was used to investigate the shift in melt interface position caused by the release of the latent heat of fusion and by finite length effects. These effects were subsequently investigated by Riquet and Durand [2], who obtained a restricted solution, and by Sukanek and Fu [3], who recently obtained a more general solution. Bartholomew and

Hellawell [4] used a one-dimensional finite element method to obtain the temperature profiles in a directionally solidified Al sample as a function of its position in the furnace, assuming steady-state conditions. Clyne [5] performed both experimental and computer analysis of the directional solidification of Al at higher translational velocities and demonstrated that for materials with high thermal conductivity there may be a significant difference between the sample pull rate and the actual growth velocity.

Fu and Wilcox [6] investigated a three-zone furnace in which the hot and cold zones were separated by a short adiabatic zone. Computer modeling using a finite difference scheme was employed, which allowed unequal heat-transfer coefficients to be considered in the hot and cold zones. It was shown that the use of an adiabatic zone significantly reduced the curvature of the isotherms between the hot and cold zones and allowed much better control over the shape of the melt interface. This benefit, however, is at the expense of some loss in gradient.

In many experiments involving small sample diameters and fairly conductive materials, a one-dimensional analysis is quite adequate for describing the conditions at the melt interface, particularly if an adiabatic zone is used. Although such an analysis obviously cannot provide information about the planarity of the interface, it can yield accurate predictions of the position of the interface and the axial gradients in the solidification region as functions of the furnace and sample parameters. This provides a useful model for furnace optimization and for selection of experimental conditions.

The one-dimensional analysis of Chang and Wilcox is extended in this work to include an adiabatic zone, different heat transfer coefficients in the hot and cold zones, change in sample material properties associated with phase change, and the inclusion of a booster heater adjacent to the adiabatic zone to provide additional control over the gradient and position of the melt interface.

ANALYSIS

The heat-flow equation for a long, thin object with uniform cross-sectional area A and perimeter p and which moves along its axis with velocity u and transfers heat laterally with an external source or sink at temperature T_1 is [7]

$$\frac{\partial^2 T}{\partial X^2} - \frac{u\rho c}{k}\frac{\partial T}{\partial X} - \frac{Hp}{Ak}(T - T_1) - \frac{\rho c}{k}\frac{\partial T}{\partial t} = 0 , \tag{1}$$

where H is the heat-transfer coefficient, $k/\rho c$ is the thermal diffusivity, and k is the thermal conductivity. For a cylindrical rod, the heat-transfer term becomes

$$\frac{Hp}{Ak} = \frac{2H}{a_o k} , \tag{2}$$

where a_o is the sample radius.

It is convenient to introduce dimensionless coordinates, $x = X/a_o$. The heat transfer can be characterized by a dimensionless Biot number,

$$B_i = \frac{Ha_o}{k} \tag{3}$$

and the motion of the sample can be described by a dimensionless Peclét number

$$P_e = \frac{\rho c a_o u}{k} . \tag{4}$$

The dimensionless heat-flow equation for steady state becomes

$$\frac{d^2T}{dx^2} - P_e \frac{dT}{dx} - 2B_i (T - T_1) = 0 \, , \tag{5}$$

and the general solution is

$$T = T_1 + C \exp(\alpha^* x) + D \exp(-\alpha^* x) \quad , \tag{6}$$

where

$$\alpha^* = \frac{\sqrt{4\alpha^2 + P_e^2} \pm P_e}{2}$$

and

$$\alpha = \sqrt{2B_i} \; ; \; B_i > 0 \; .$$

If $B_i = 0$,

$$T = A + C \exp(P_e x) \tag{7}$$

To isolate various aspects of the problem, several simplified cases will be considered. First, the effect of the motion of the rod will be investigated in a three-zone furnace for a rod sufficiently long that end effects can be neglected. Next, the end effects will be investigated for a motionless rod. Finally, the addition of a fourth zone, an independently controlled booster heater between the main heater and the adiabatic zone, will be evaluated for its ability to increase the gradient in the sample at the melt interface and to control the position of the interface.

Case I: Effect of Sample Translation

The general solutions for an infinite rod in a three-zone furnace are:

$$T_L(x) = T_H - D \exp[\beta^*(x + x_1)] \qquad ; -\infty < x \leq -x_1$$

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$$T_L(x) = A + B \exp(P_L x) \qquad ; -x_1 \le x \le x_o$$

$$T_S(x) = A^* + B^* \exp(P_S x) \qquad ; x_o \le x \le x_1 \tag{8}$$

$$T_S(x) = T_C + C \exp[-\alpha^*(x - x_1)] \qquad ; x_1 \le x \le \infty$$

where

$$\alpha^* = \frac{\sqrt{4\alpha^2 + P_S^2} - P_S}{2} \qquad \alpha = \sqrt{2B_C}$$
$$\beta^* = \frac{\sqrt{4\beta^2 + P_L^2} + P_L}{2} \quad ; \qquad \beta = \sqrt{2B_H} \quad ; \tag{9}$$

subscripts L and S denote liquid and solid regions, respectively, and B_H and B_C are the Biot numbers in the hot and cold zones. Unless otherwise noted in the following, all lengths will be expressed in terms of sample radii. The length of the adiabatic zone, $L_A = 2x_1$. The position of the melt interface is x_o and is presumed to be in the adiabatic zone since this tends to yield a planar interface.

The equations must be solved simultaneously for seven unknowns, A, B, A*, B*, C, D and x_o. Four constraints are provided by requiring T_L and T_L' to be continuous at $-x_1$ and T_s and T_s' to be continuous at x_1. The remaining three conditions are provided by requiring $T_L(x_o) = T_S(x_o) = T_M$ and

$$-k_L \left.\frac{\partial T_L}{\partial x}\right)_{x_o} + L_f = -k_S \left.\frac{\partial T_S}{\partial x}\right)_{x_o} , \tag{10}$$

where L_f is the latent heat of fusion term

$$L_f = \rho_L \, a_o \, u \, \Delta H_f = \frac{P_L \, k_L \, \Delta H_f}{c_L} \tag{11}$$

and ΔH_f is the heat of fusion.

and T_M is the melting temperature.

The position of the interface requires the solution of the transcendental equation

$$\frac{k_L P_L (T_H - T_M) \exp(P_L x_o)}{\exp(-P_L X_1)\left(\frac{P_L}{\beta^*} - 1\right) + \exp(P_L x_o)} + L_f = \frac{k_S P_S (T_M - T_c) \exp(P_S x_o)}{\exp(P_S x_1)\left(\frac{P_S}{\alpha^*} + 1\right) - \exp(P_S x_o)} \quad . \tag{12}$$

The remaining terms may be evaluated

$$B = -\frac{T_H - T_M}{\exp(-P_L x_1)\left(\frac{P_L}{\beta^*} - 1\right) + \exp(P_L x_o)} \tag{13}$$

$$B^* = -\frac{T_M - T_c}{\exp(+P_S x_1)\left(\frac{P_S}{\alpha^*} + 1\right) - \exp(P_S x_o)} \tag{14}$$

$$A = T_H + B \exp(-P_L x_1)\left(\frac{P_L}{\beta^*} - 1\right) \tag{15}$$

$$A^* = T_c - B^* \exp(P_S x_1)\left(\frac{P_S}{\alpha^*} + 1\right) \tag{16}$$

$$C = -\frac{P_S B^* \exp(P_S x_1)}{\alpha^*} \tag{17}$$

$$D = -\frac{P_L B \exp(-P_L x_1)}{\beta^*} \tag{18}$$

If P_S and P_L are small so that $P_S x_o \simeq P_L x_o << 1$, the gradients in the sample at x_o may be found from

$$G_L(x_o) = P_L\, B \exp(P_L x_o) = -\frac{(T_H - T_M)\,(1 + P_L x_o + O(P_L^2))}{x_1 + 1/\beta^* + x_o - P_L\left(\frac{x_1^2}{2} - \frac{x_o^2}{2} + \frac{x_1}{\beta^*}\right) + O(P_L^2)} \tag{19}$$

and

$$G_S(x_o) = P_S\, B^* \exp(P_S x_o) = -\frac{(T_M - T_C)\,(1 + P_S x_o + O(P_L^2))}{x_1 + 1/\alpha^* - x_o + P_S\left(\frac{x_1^2}{2} - \frac{x_o^2}{2} + \frac{x_1}{\alpha^*}\right) + O(P_S^2)} \tag{20}$$

In the limit $P_L = P_S = 0$, the position of the melt interface can be obtained by equating $k_S G_S(x_o) = k_L G_L(x_o)$, which yields

$$x_o = \frac{k_L\,(T_H - T_M)(x_1 + 1/\alpha) - k_S\,(T_M - T_C)(x_1 + 1/\beta)}{k_L\,(T_H - T_M) + k_S\,(T_M - T_C)} \tag{21}$$

and

$$G_L = -\frac{T_H - T_M + k_S/k_L\,(T_M - T_C)}{L_A + 1/\alpha + 1/\beta}\,. \tag{22}$$

Case II: Investigation of End Effects

To assess the importance of end effects, the complications introduced by the motion of the rod will be suppressed by setting the Peclet numbers to zero, and the rod will be inserted a finite distance L into the hot zone (see Figure 1).

The solution to the heat flow equation in the hot zone is

$$T_L(x) = T_H - D \exp[\beta(x + x_1)] + B \exp[-\beta(x - x_1)] ; -x_3 \le x \le -x_1 \quad . \tag{23}$$

In the adiabatic zone for $P \to 0$, the heat-flow equation reduces to $T'' = 0$ and the solution is

$$T_L(x) = T_o + G_L x \quad ; \quad -x_1 \le x \le x_o \tag{24}$$

and

$$T_S(x) = T_o^* + G_S x \; ; \; x_o \le x \le x_1 \quad . \tag{25}$$

As before, it is tacitly assumed that the interface is located in the adiabatic zone.

The fourth equation is as in Case I,

$$T_S(x) = T_C + C \exp[-\alpha(x - x_1)] \quad ; \quad x_1 \le x \le \infty \tag{26}$$

The interfacial conditions at $-x_1$, x_o and x_1 together with the requirement that $T(x_o) = T_M$ provide seven of the eight equations needed to specify the unknown coefficients. The final boundary condition is imposed by the heat transfer to the end of the rod at $-x_3$.

$$\left(\frac{\partial T_L}{\partial x}\right)_{-x_3} = -B_H^* \quad (T_H - T_L(-x_3)) \quad , \tag{27}$$

where $B_H^* = H^* a_o/k$ and H^* is the heat-transfer coefficient between the end of the rod and the furnace.

The solutions are:

$$G_L = - \frac{T_H - T_M + k_S/k_L\ (T_M - T_C)}{L_A + 1/\alpha + 1/\beta\ F(L)}$$

$$G_S = k_L\ G_L/k_S$$

$$x_o = \frac{k_L\ (T_H - T_M)(x_1 + 1/\alpha) - k_S\ (T_M - T_C)(x_1 + 1/\beta\ F_{(L)}}{k_L\ (T_H - T_M) + k_S\ (T_M - T_C)}$$

$$T_o = T_M - G_L\ x_o$$

$$T_o{}^* = T_M - G_S\ x_o$$

$$C = -G_S/\alpha$$

$$B = \frac{G_L \exp\ (-\beta L)}{\beta \left[\left(\frac{1 + B_H{}^*/\beta}{1 - B_H{}^*/\beta}\right) \exp\ [\beta(L + L_A)] - \exp\ [-\beta(L - L_A)]\right]}$$

$$D = - \frac{G_L}{\beta \left[1 - \left(\frac{1 - B_H{}^*/\beta}{1 + B_H{}^*/\beta}\right) \exp\ (-2\beta L)\right]}$$

$$F\ (L) = \frac{(1 + B_H{}^*/\beta) \exp\ (\beta L) + (1 - B_H{}^*/\beta) \exp\ (-\beta L)}{(1 + B_H{}^*/\beta) \exp\ (\beta L) - (1 - B_H{}^*/\beta) \exp\ (-\beta L)}$$

Case III. Effect of Booster Heater

The effects of an additional independently heated zone to sharpen the gradient in the sample and to provide additional control of the interface position will be investigated without the complications of sample motion or end effects. The heat flow equations are:

$$
\begin{aligned}
T_L(x) &= T_H - D \exp \beta (x + x_3) && ; \ -\infty < x \leq -x_3 \\
T_L(x) &= T_B + A \exp [\beta(x + x_2)] + B \exp [-\beta(x + x_2)] && ; \ -x_3 \leq x \leq -x_1 \\
T_L(x) &= T_o + G_L x && ; \ -x_1 \leq x \leq x_o \qquad (37) \\
T_S(x) &= T_o^* + G_S x && ; \ x_o \leq x \leq x_1 \\
T_S(x) &= T_C + C \exp [-\alpha(x - x_1)] && ; \ x_1 \leq x \leq \infty ,
\end{aligned}
$$

where the length of the adiabatic zone is $L_A = 2x_1$, as before, and the booster heater is centered at $-x_2$ and has length L_B (see Figure 2).

This set of equations contains nine unknowns. Interfacial boundary conditions at $-x_3$, $-x_1$, x_o, and x_1 supply eight of the necessary constraining relations, and the requirement that $T(x_o) = T_M$ supplies the ninth equation. Again, it is assumed that the interface is located in the adiabatic zone. The solution of this set yields the following relations:

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$$G_L = -\left[\frac{(T_B - T_H)\,[1 - \exp(-\beta L_B)] + (T_H - T_M) + k_S/k_L\,(T_M - T_C)}{L_A + 1/\beta + 1/\alpha}\right] \tag{38}$$

$$x_o = \frac{(k_S/k_L)\,(T_M - T_C) + G_L\,(x_1 + 1/\alpha)}{G_L} \tag{39}$$

$$G_S = k_L\,G_L/k_S \tag{40}$$

$$C = -G_S/\alpha \tag{41}$$

$$B = \frac{(T_H - T_B)}{2}\exp(-\beta L_B/2) \tag{42}$$

$$A = \frac{B\exp(-\beta L_B/2) + G_L/\beta}{\exp(\beta L_B/2)} \tag{43}$$

$$D = B\exp(\beta L_B/2) - A\exp(-\beta L_B/2) \tag{44}$$

$$T_o = T_M - G_L\,x_o$$

$$T_o^* = T_M - G_S\,x_o \tag{45}$$

Estimation of Effective Heat Transfer Coefficients

To use the analytical model as a predictive tool, it is necessary to estimate the effective heat transfer coefficients in the hot and cold zones. Also, since the simplified analysis considers a homogeneous sample, some provision must be made to account for the presence of the ampoule. If the axial heat flow in the ampoule is very small compared with that conducted by the sample, the presence of the ampoule can be included simply as an added resistance in the heat transfer between the sample and the furnace wall. A more general technique is to modify the thermal properties of the sample by defining an effective conductivity as the area weighted average of the sample and ampoule thermal conductivities. The effective Peclét numbers may be found by dividing the area weighted average heat carried by the sample plus ampoule by the effective conductivity. Since the ampoule does not contribute to the heat of fusion, the effective latent heat is the sample latent heat times the ratio of sample area to total area.

At high temperatures, the heat transfer in the hot zone is dominated by radiation. The radiation heat transfer coefficient is given by

$$H_{rad}(x) = \frac{\dot{Q}(x)}{T_H - T_L(x)} = \frac{\sigma F_e \left[T_H^4 - T_L^4(x)\right]}{T_H - T_L(x)} , \qquad (46)$$

where $\dot{Q}(x)$ is the heat flux transmitted at position x, F_e is

$$F_e = \frac{1}{1/\varepsilon^* + a_o/a_f \, (1/\varepsilon_f - 1)} , \qquad (47)$$

ε^* is the effective emissivity of the ampoule/sample combination, ε_f is the emissivity of the furnace wall, and a_f is the inside radius of the furnace muffle [8].

The heat transfer coefficient given by equation (46) is a function of position. The simplified one-dimensional analysis requires a constant value of H_{rad} that represents some type of average. The method chosen for computing this average is to require $\langle H_{rad} \rangle$ to give the same total integrated heat transfer as H_{rad} (x), i.e.,

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$$\int_{-\infty}^{-x_1} \dot{Q}(x)\, dx = \langle H_{rad} \rangle \int_{-\infty}^{-x_1} [T_H - T_L(x)]\, dx = \sigma F_e \int_{-\infty}^{-x_1} [T_H^4 - T_L(x)^4]\, dx. \tag{48}$$

Since

$$T_L(x) = T_H - D \exp [\beta^* (x + x_1)],$$

$$\langle H_{rad} \rangle = \sigma F_e \left[\frac{25}{12} T_H^3 + \frac{13}{12} T_H^2 \ T_L(-x_1) + \frac{7}{12} T_H \ T_L^2(-x_1) + \frac{1}{4} T_L^3(-x_1) \right], \tag{49}$$

where $T_L(-x_1) = T_H - D$ and is the temperature at the boundary between the hot zone and the adiabatic zone. This is not known ab initio but may be determined by an iterative process.[1]

In many cases the sample is enclosed in a quartz ampoule which has near unity transmission to some cutoff wavelength, λ_c, and is nearly opaque for $\lambda > \lambda_c$. The effective emissivity of the ampoule/sample combination may be estimated using the technique suggested by Holland [9],

$$\varepsilon^* = 0.95 \ [1 - f(\lambda_c)(1 - \varepsilon_s)] \tag{50}$$

where the 0.95 accounts for the surface reflectivity, ε_s is the emissivity of the sample material inside the quartz ampoule for wavelengths shorter than λ_c, and $f(\lambda_c)$ is the fraction of radiation emitted at T_H which is shorter than λ_c. For metal-like samples, ε_s is usually small and the long wavelength absorption in the quartz ampoule is the dominant mode of heat transfer into the sample. For such cases axial radiant heat transfer in the quartz ampoule is negligible.

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[1] As a first estimate, $T_L\ (-x_1) \approx (T_H + T_M)/2$.

A similar treatment may be employed in the cold end by substituting T_c for T_H and $T_s(x_1)$ for $T_L(-x_1)$. In this case $f(\lambda_c)$ is computed for $T_s(x_1)$.

If there is a fluid such as a low-pressure gas in the furnace, its conductive heat transfer is given by

$$H_{cond} = \frac{k_G}{a_o \ln (a_f/a_o)} , \tag{51}$$

where k_G is the conductivity of the fluid.

If flowing gas is used for heat extraction, the heat transfer coefficient for forced convection is estimated from the work of Chen, Hawkins, and Solberg [10],

$$H_{conv}(x) = 1.02 \frac{k_G}{d} \left(\frac{\rho d v}{\mu}\right)^{0.45} \left(\frac{c_p \mu}{k_G}\right)^{0.33} \left(\frac{a_f}{a_o}\right)^{0.8} \left(\frac{d}{x}\right)^{0.4} , \tag{52}$$

where v is the velocity, ρ is the density, c_p is the heat capacity, μ is the dynamic viscosity, and k_G is the conductivity of the gas; d is the equivalent diameter given by $2 (a_f - a_o)$, and x is the position along the flow. Again, this heat transfer coefficient depends on position; and an average value must be found for use in the simplified model. This average is

$$\langle H_{conv} \rangle = \frac{1}{L} \int_o^L H_{conv}(x) \, dx = \frac{H_{conv}(L)}{.6} , \tag{53}$$

where H_{conv} (L) is equation (52) evaluated at x = L, where L is the length of the sample in the furnace zone.

In the absence of forced convection, the heat transfer from natural convection in a vertical furnace may be estimated by replacing v in equation (52) by $v = [g\beta \Delta T L]^{\frac{1}{2}}$, where g is the acceleration of gravity, β is the coefficient of thermal expansion, and ΔT is the average temperature difference between the ampoule and furnace wall.

RESULTS

The one-dimensional model described in this analysis was applied to a case that had been computed by a sophisticated two-dimensional heat-transfer analysis of a development furnace designed for use on the Space Shuttle as part of the NASA Materials Processing in Space program. The two-dimensional analysis was done with the System Improved Numerical Difference Analyzer code (SINDA) [10] which represents the furnace by 580 nodes and 1420 conductors, and represents the sample plus ampoule by 5 nodes in the radial direction and 40 nodes in the axial direction. View factors are computed for radiation exchange between each element on the surface of the sample and all elements in the furnace within the field of view.

The furnace consists of a 27.8 cm hot zone, an independently controlled 1.96 cm booster heater zone, a 2.03 cm adiabatic zone, and a 24.5 cm cold zone. Heat extraction and thermal control in the cold zone are accomplished by flowing temperature-controlled He gas along the sample.

The effective heat transfer coefficients and Biot numbers were estimated by the method outlined in the previous section. See the appendix for the numerical calculations. The thermal profiles of an infinite Mn-Bi/Bi eutectic sample were computed for $T_H = 450°C$, $T_C = 40°C$, and $T_B = 450°C$ and 500°C. These are shown in Figure 3 together with similar temperature profiles computed using the SINDA code. Reasonably good agreement is obtained in the hot and cold zones, and the gradients at the solidification interface are in fairly close agreement. The major discrepancy between the two computation methods is in the position of the solidification interface. The interface locations predicted by SINDA are shifted approximately 3 mm closer to the cold zone than are those predicted by the one-dimensional model. There are several possible reasons for this.

First, the simplified one-dimensional model assumes a perfectly adiabatic zone. The SINDA allows some heat transfer in the adiabatic zone from radiation losses and conduction from the hot (or booster heater) zone. Another possible reason for this shift is the fact that the simple model uses a constant average heat transfer coefficient in the hot/booster heater zone. The inside diameter of the booster heater in the furnace in question is smaller than the diameter of the hot zone; hence, the conductive heat transfer will be underestimated in this zone by the simplified model.

Despite these shortcomings, the simplified model can be used to investigate effects of varying sample and furnace parameters. For example, the effect of sample insertion length into the hot zone may be seen in Figure 4. As the sample is withdrawn from the hot zone, the interface shifts toward the heater. This effectively increases the solidification velocity above the pull rate. It may also be seen that the heat transfer coefficient into the end of the sample makes only a small difference in the thermal profile and that the thermal field in the sample is almost fully developed after insertion lengths of $a_o/\sqrt{2B_H}$.*

*For finite samples whose "heat transfer length", $\mathcal{L}$, as defined by Sukanek (ω_c in Riquet and Durand notation) is >> 1; this is equivalent to requiring the fraction immersed in the hot zone to be > $1/\mathcal{L}$.

The effect of sample translation is shown in Figure 5. As velocity is increased, the interface is shifted toward the cold zone. Note that the gradient in the melt is less affected by translation than the gradient in the solid. Also note that for the case of Mn-Bi/Bi eutectic, the release of latent heat of fusion is responsible for approximately half of the interface shift.

Optiumum Length for Booster Heater Zone

It can be seen from equation (38) that the magnitude of the gradient can be increased for a given T_B by increasing L_B. However, if L_B is made long, it has virtually the same effect as simply increasing T_H. In many cases, the upper limit of T_H is fixed by other considerations, such as melting point of the ampoule or vapor pressure of the sample, and temperatures higher than T_H in the sample cannot be tolerated. The function of the booster heater is to reduce the roll-off in temperature near the adiabatic zone without exceeding T_H anywhere in the sample. This requirement places a limitation on the length L_B that is a function of the maximum T_B that can be supplied by the booster heater.

The requirement that T_H not be exceeded anywhere in the sample can be enforced by keeping $D \geq 0$. This implies from equation (44) that

$$B \exp(\beta L_B) \geq A \exp(-\beta L_B/2) \quad . \tag{54}$$

The highest T_B that can be used for a given L_B without overheating the sample is obtained by setting $D = 0$ and using equations (42) and (43),

$$(T_B - T_H)_{max}\, \beta \sinh \beta L_B = -G_L \quad . \tag{55}$$

Equating this to (38),

$$(T_B - T_H)_{max} = \frac{T_H - T_M + k_S/k_L\ (T_M - T_C)}{\beta(L_A + 1/\alpha)\ \sinh\ \beta L_B + \cosh\ \beta L_B - 1} \quad . \tag{56}$$

Substituting this into equation (55), the maximum gradient that can be achieved for a given L_B with no restriction on T_B is

$$|G_L|_{max} = \frac{[T_H - T_M + k_S/k_L\ (T_M - T_C)]\beta\ \sinh\ \beta L_B}{\beta(L_A + 1/\alpha)\ \sinh\ \beta L_B + \cosh\ \beta L_B - 1} \quad . \tag{57}$$

For $\beta L_B >> 1$,

$$|G_L|_{max} \cong \frac{T_H - T_M + k_S/k_L\ (T_M - T_C)}{L_A + 1/\alpha + 1/\beta} \quad , \tag{58}$$

which is the gradient given by eq. (22) for the three-zone configuration. This comes about because eq. (56) forces $T_B \to T_H$ as $\beta L_B >> 1$ to avoid overheating the sample. On the other hand, for $\beta L_B << 1$,

$$|G_L|_{max} \cong \frac{T_H - T_M + k_S/k_L\ (T_M - T_C)}{L_A + 1/\alpha + L_B/2} \quad , \tag{59}$$

and the maximum gradient can be obtained by $L_B \to 0$. This, however, requires $T_B \to \infty$. Since $T_{B(max)}$ is fixed by practical considerations, there is an optimum length for the booster heat that depends on $T_{B(max)}$ and the sample to be processed. This L_B(optimum) is the value of L_B for which the maximum gradient limited by heater temperature, eq. (33) intersects the maximum gradient limited by sample overheating considerations, eq. (56). This value is

$$L_{B(opt)} = 1/\beta\ \ln\left(C_1 + \sqrt{C_1^{\ 2} + C_2}\right) \quad , \tag{60}$$

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where

$$C_1 = \frac{T_{B(max)} - T_M + k_S/k_L\ (T_M - T_C)}{\beta(L_A + 1/\alpha + 1/\beta)(T_{B(max)} - T_H)} \tag{61}$$

and

$$C_2 = \frac{L_A + 1/\alpha - 1/\beta}{L_A + 1/\alpha + 1/\beta} \quad . \tag{62}$$

The previous optimization assumed that the cold-end temperature T_C remained constant. As T_B is increased, the solidification front x_o is driven toward the cold zone. If the cold-end performance permits, the T_C may be lowered to maintain the position of the interface near the center of the adiabatic zone. This also increases the maximum achievable gradient.

From eq. (39), the interface can be maintained at $x = 0$ by setting

$$k_S/k_L\ (T_M - T_C) = -G_L\ (x_1 + 1/\alpha) \ . \tag{63}$$

Putting this into eq. (38) yields

$$G_L = -\left[\frac{(T_B - T_H)\ [1 - \exp\ (-\beta L_B)] + T_H - T_M}{x_1 + 1/\beta}\right] \tag{64}$$

Employing eq. (55) to prevent sample overheating provides the maximum value for $T_B - T_H$.

$$(T_B - T_H)_{max} = \frac{T_H - T_M}{\beta x_1\ \sinh\ \beta L_B + \cosh\ \beta L_B - 1} \quad . \tag{65}$$

Inserting this into equation (55) yields

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$$|G_L|_{max} = \beta(T_H - T_M)\left[\frac{\sinh \beta L_B}{\beta x_1 \sinh \beta L_B + \cosh \beta L_B - 1}\right] . \quad (66)$$

If L_B is less than the optimum length, the performance is limited by booster heater performance and G_L is given by eq. (64). As before, the optimum length for L_B is given by the intersection of eqs. (64) and (66), which is

$$L_{B(opt)} = \frac{1}{\beta}\log_e\left[\frac{1 + \Theta + \sqrt{1 + 2\Theta + \beta^2 x_1^{\,2}\,\Theta^2}}{(1 + \beta x_1)\Theta}\right] , \quad (67)$$

where

$$\Theta = (T_{B(max)} - T_H) / (T_H - T_o) . \quad (68)$$

The required cold-end temperature to position the interface at $x = 0$ is obtained from equation (63) and becomes

$$T_{C(req'd)} = G_L\,(x_1 + 1/\alpha)\,(k_L/k_S) + T_M . \quad (69)$$

The effect of optimizing the booster-heater length is shown in Figure 6. In this case, the sample is $Pb_{.8}Sn_{.2}Te$. It is assumed that the booster heater cannot tolerate more than 1200°C and that the booster heater cannot be operated above 1600°C. As may be seen in Figure 6, the maximum allowable booster-heater temperature and gradient increase as the booster-heater length is shortened until the maximum booster operating temperature is reached. Beyond this point, further decrease in booster heater length results in lower gradients as the booster heater loses its effectiveness. As would be expected, lowering the cold-end temperature to compensate for the booster heater in maintaining a stationary solidification interface will give a higher gradient than operating with fixed T_C. This can be seen more clearly in Figure 7, which compares the axial thermal profiles in a sample with no booster heater and T_C set to position the interface at $x = 0$, with profiles for an optimized booster heater operating a 1600°C and fixed cold-end temperature and also with profiles for an optimized booster heater and T_C adjusted to position the melt interface in the center of the adiabatic zone.

The booster heater provides another degree of freedom in positioning the solidification interface independently of the hot and cold zone temperatures, which may be fixed by other considerations. Differentiating eq. (39) with respect to T_B yields

$$\frac{\partial x_o}{\partial T_B} = \frac{k_S\ (T_M - T_C)[1 - \exp\ (-\beta L_B)]}{k_L\ G_L{}^2\ (L_A + 1/\alpha + 1/\beta)} \quad . \tag{70}$$

Since the sign of the derivative is positive, an increase in T_B will shift the melt interface toward the cold zone. The booster heater temperature may be selected to locate the solidification isotherm at a position of optimum planarity, or this temperature may be programmed to maintain the position of the isotherm as the sample is withdrawn from the furnace and to compensate for T_M changes as a result of compositional effects during solidification.

SUMMARY

A relatively simple one-dimensional thermal model of the Bridgman growth process has been developed which is applicable to the growth of small diameter ($\leq$ 1 cm) samples with conductivities similar to those of metallic alloys. Although the model contains some idealized assumptions that limit its ability to match actual thermal profiles exactly, it is useful for predicting thermal gradients, estimating solidification interface position, and analyzing effects of sample translation and sample insertion length.

The fact that analytical results are available is particularly helpful in performing furnace design trade studies and for inverting measured data to obtain furnace characteristics. Also, sensitivity analyses of furnace performance in terms of furnace and sample parameters may be accomplished by analytical techniques rather than by numerical analysis. This was used to determine the optimum length of the booster heater to produce a maximum thermal gradient in the sample for a given set of design constraints.

ACKNOWLEDGMENT

The author wishes to express his appreciation for the technical assistance of Ms. Ernestine Cothran in developing this analytical model.

APPENDIX

In the case analyzed by SINDA, $T_H = 450°C$, $T_C = 40°C$ and $T_M = 271.5$. The Mn Bi/Bi eutectic was approximated thermally by pure Bi since this is a very low volume fraction eutectic. The thermal conductivities were taken as $k_L = 0.124$ watt/cm/K and $k_S = 0.072$ watt/cm/K. The quartz ampoule was 1.2 cm O.D. and 1.0 cm I.D. Thermal conductivity of the quartz was assumed to be 0.020 watt/cm/K. Effective conductivities are the area weighted average, or $k_L(\text{eff}) = 0.0922$ watt/cm/K and $k_S(\text{eff}) = 0.0561$ watt/cm/K. The effective Peclét numbers are given by $(\rho c)\text{eff}\ a_o u/k(\text{eff})$. Using $\rho = 10.05$ gm/cm^2 for Bi and 2.3 gm/cm^3 for quartz, $c = 0.1463$ J/gm for Bi and 0.493 J/gm for quartz, $P_L(\text{eff}) = 8.90$ u and $P_S(\text{eff}) = 14.63$ u. Since the ampoule does not contribute to the heat of fusion, $\Delta H\ (\text{eff}) = 50.16\ (.5/.6)^2 = 34.83$ Joules/gm.

Cutoff wavelength λ_c for the quartz was taken to be 3.7 mm. For $T_H = 723K$, $f(\lambda_c) = 0.20$, and for $T_c = 313K$, $f(\lambda_c) = 0.0015$. The ε_s was taken to be 0.05. The effective sample/ampoule emissivity is therefore $\varepsilon_H^* = 0.7695$ and $\varepsilon_s^* = 0.9486$. Taking the inside diameter of tantalum muffle to be 5.2 cm with an $\varepsilon_f = 0.3$, the F_e term is 0.5441 for the hot zone and 0.6279 for the cold zone. The average radiation heat transfer coefficients become

$$\langle H_H \text{rad}\rangle = 0.00445 \text{ watt/cm}^2\text{/K}$$

$$\langle H_C \text{rad}\rangle = 0.000557 \text{ watt/cm}^2\text{K} \quad .$$

Heat extraction in the cold zone is accomplished by flowing He. Using a 4 lb/hr flow rate through the cold zone (a_f = 1.77 cm, a_o = 0.6 cm), the heat transfer coefficient used in SINDA is 23.36 $x(ft)^{-0.4}$ BTU/hr/ft^2/°F. For a 25 cm long sample inserted half its length into the cold zone, the average heat transfer coefficient is 58.9 BTU/hr/ft^2/°F or 0.0312 watt/cm^2/K.

A stagnant region of He will also be present in the hot end. Since the furnace was designed for low-gravity operation, convective heat transfer was not analyzed. The conductivity of He at 450°C is taken as 0.0023 watts/cm/K, and the conductive heat transfer coefficient is therefore 0.00261 watt/cm^2/K.

The total effective heat transfer coefficient is the sum of H(rad) H(cond) and H(conv). The effective Biot number is the total effective heat transfer coefficient multiplied by the ampoule radius divided by the effective conductivity. The values are:

H_H = 0.00706 watt/cm^2/K, B_H = 0.04594

H_C = 0.03176 watt/cm^2/K, B_C = 0.3396 .

REFERENCES

[1] C. E. Chang and W. R. Wilcox, J. Crystal Growth 21 (1974) 135.

[2] J. P. Riquet and F. Durand, J. Crystal Growth 33 (1976) 303.

[3] P. C. Sukanek and T. W. Fu, "Low Peclét Number Directional Solidification by the Bridgman-Stockbarger Method, "Second Congress of Chemical Engineering, Montreal, Oct. 1981.

[4] D. M. L. Bartholomew and A. Hellawell, J. Crystal Growth 50 (1980) 453.

[5] T. W. Clyne, J. Crystal Growth 50 (1980) 684.

[6] T. W. Fu and W. R. Wilcox, J. Crystal Growth 48 (1980) 416.

[7] H. C. Carslaw and J. C. Jaeger, Conduction of Heat in Solids, 2nd ed. (Oxford, 1969).

[8] A. I. Brown and S. M. Marco, Introduction to Heat Transfer, McGraw-Hill, New York (1958).

[9] L. R. Holland, J. Crystal Growth 49 (1980) 426.

[10] C. Y. Chen, G. A. Hawkins, and H. L. Solberg, ASME Trans., 68 (1946) 99.

[11] J. P. Smith, SINDA Users' Manual, TRW Systems Report No. 14690-H001-R0-00, April 1971. NASA Contract NAS9-10435.

Figure Captions

Figure 1. Furnace/sample configuration showing coordinate system used to investigate end effects.

Figure 2. Furnace/sample configuration showing coordinate system used to investigate the effects of a booster heater.

Figure 3. Comparison of thermal profiles for a stationary Mn Bi/Bi eutectic sample computed with the simplified one-dimensional model with those computed by the SINDA code for $T_B = T_H$ and $T_B = T_H + 50°C$.

Figure 4. Effect of sample insertion length on thermal profile for a stationary Mn Bi/Bi sample in a furnace with $T_B = T_H$.

Figure 5. Effect of sample translation of thermal profiles for an infinite sample moving at 0, 10, 20, 30 cm/hr in a furnace with $T_B = T_H$.

Figure 6. Effect of booster heater length on maximum gradient obtainable in $Pb_{.8}Sn_{.2}Te$ sample without exceeding sample temperature of 1200°C. As heater length is shortened, the allowable booster heater temperature is increased (with a concomitant increase in thermal gradient) until the upper limit imposed by heater materials is reached (assumed in this case to be 1600°C). At shorter lengths, the sample gradient is limited by booster heater performance. The optimum length for the booster heater is the intersection of these two curves.

Figure 7. Thermal profiles in $Pb_{.8}Sn_{.2}Te$ with optimized booster heater analyzed in Figure 3. T_{C1} was chosen to position the solidification interface at $x_o = 0$ for $T_B = T_H$. The effect of

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[7] H. C. Carslaw and J. C. Jaeger, Conduction of Heat in Solids, 2nd ed. (Oxford, 1969).

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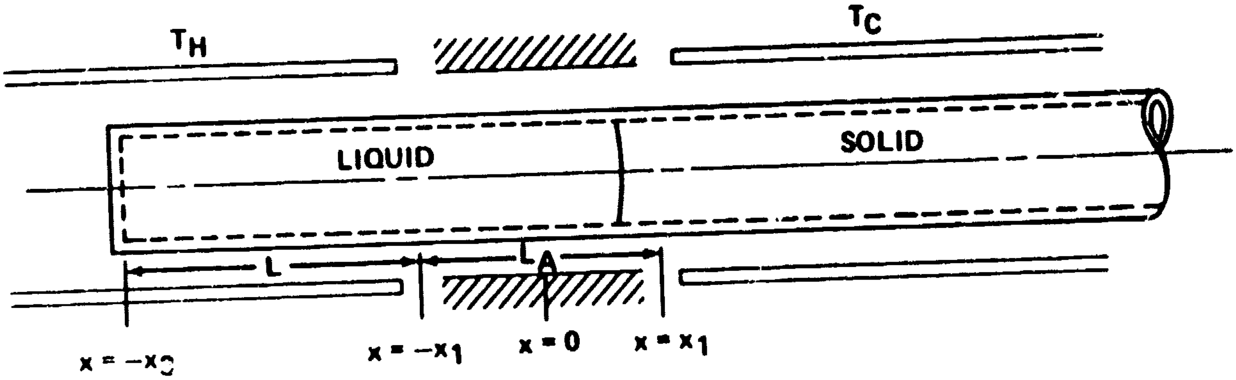

FIGURE 1

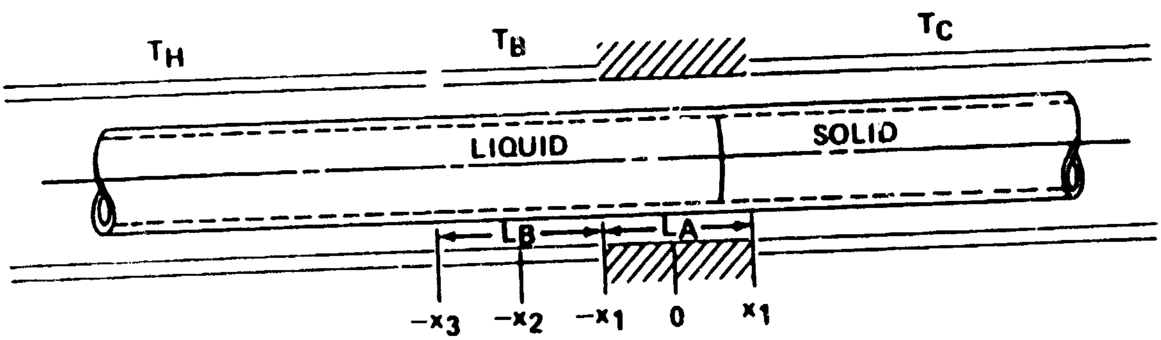

FIGURE 2

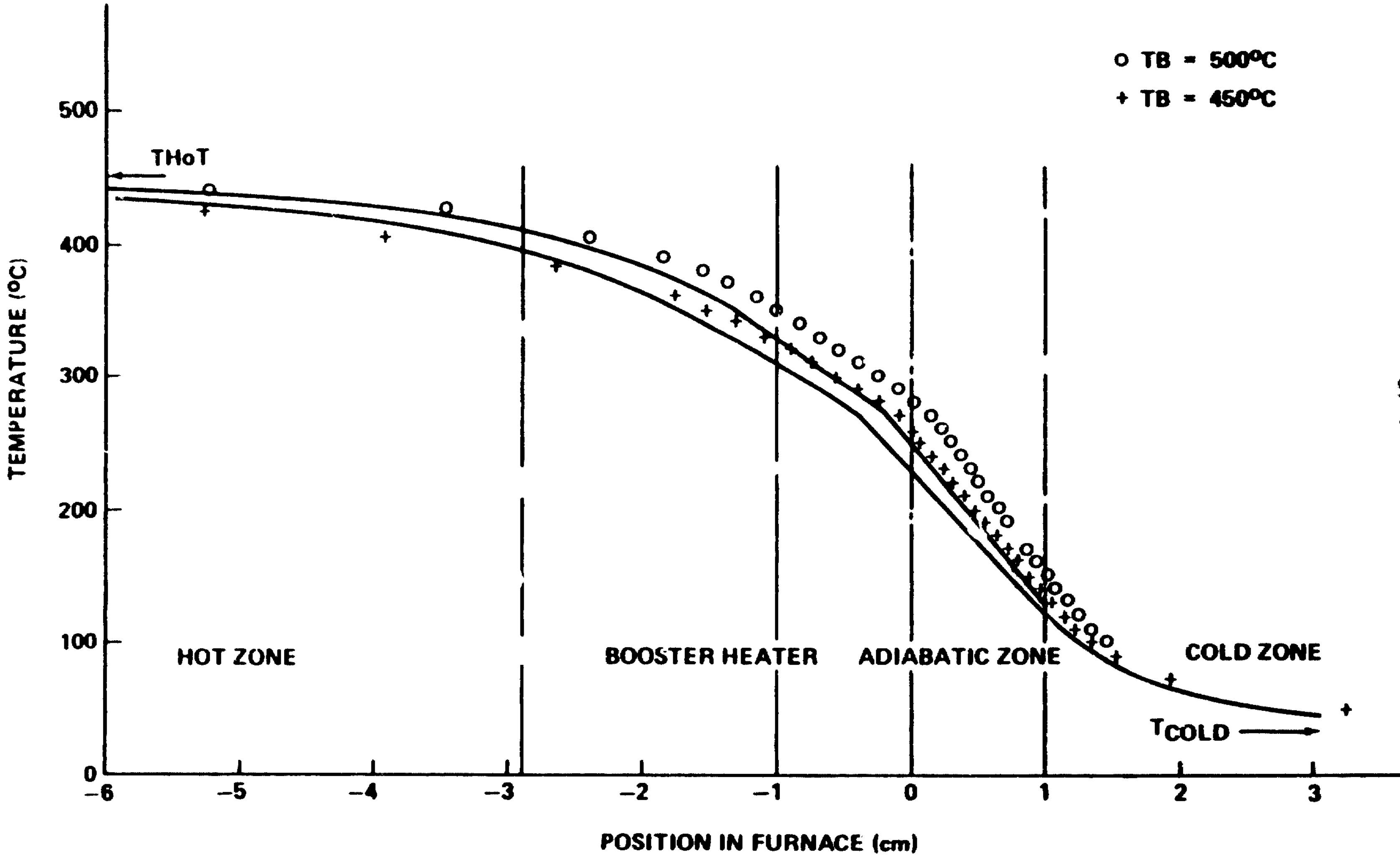

FIGURE 3

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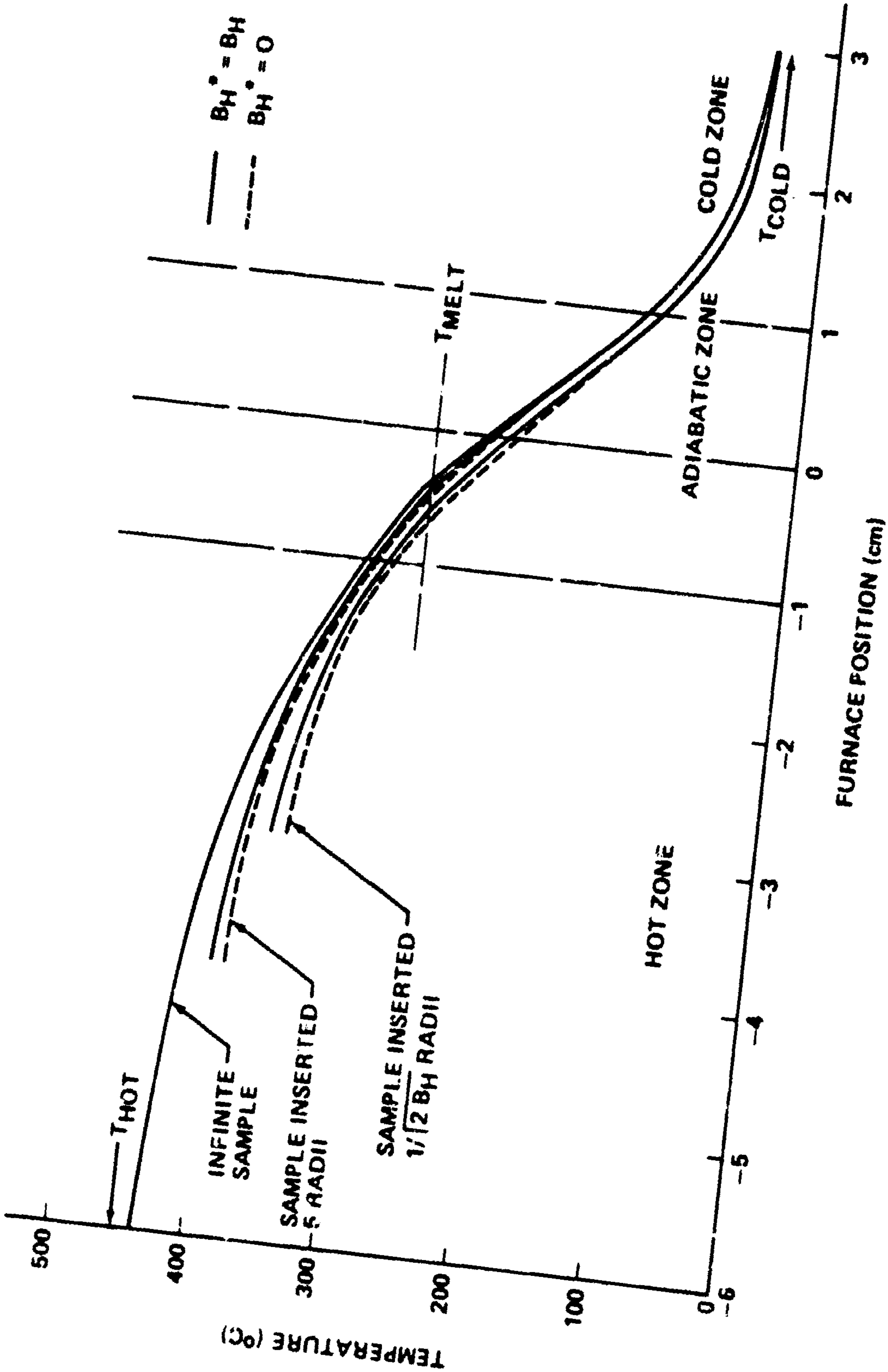

FIGURE 4

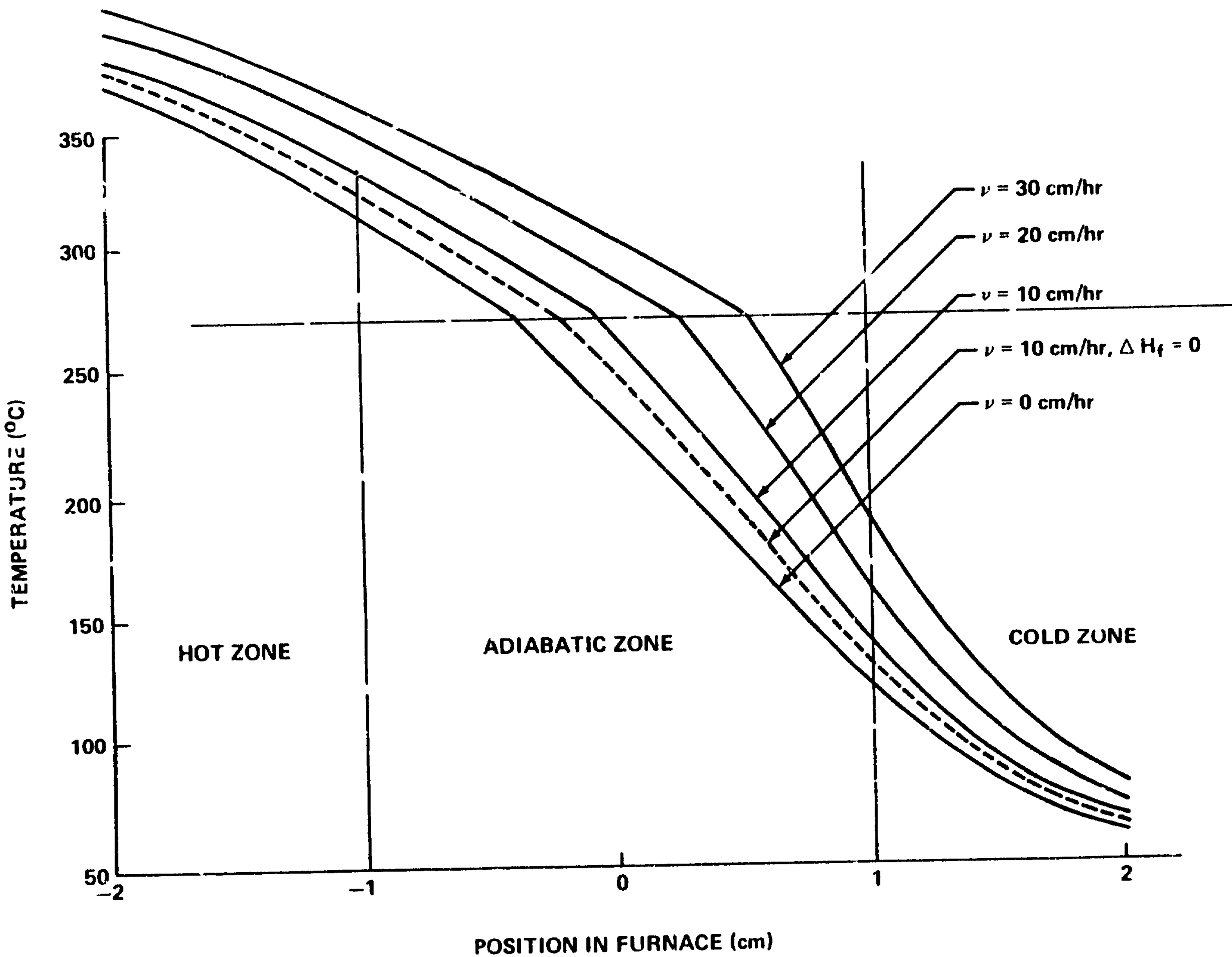

FIGURE 5

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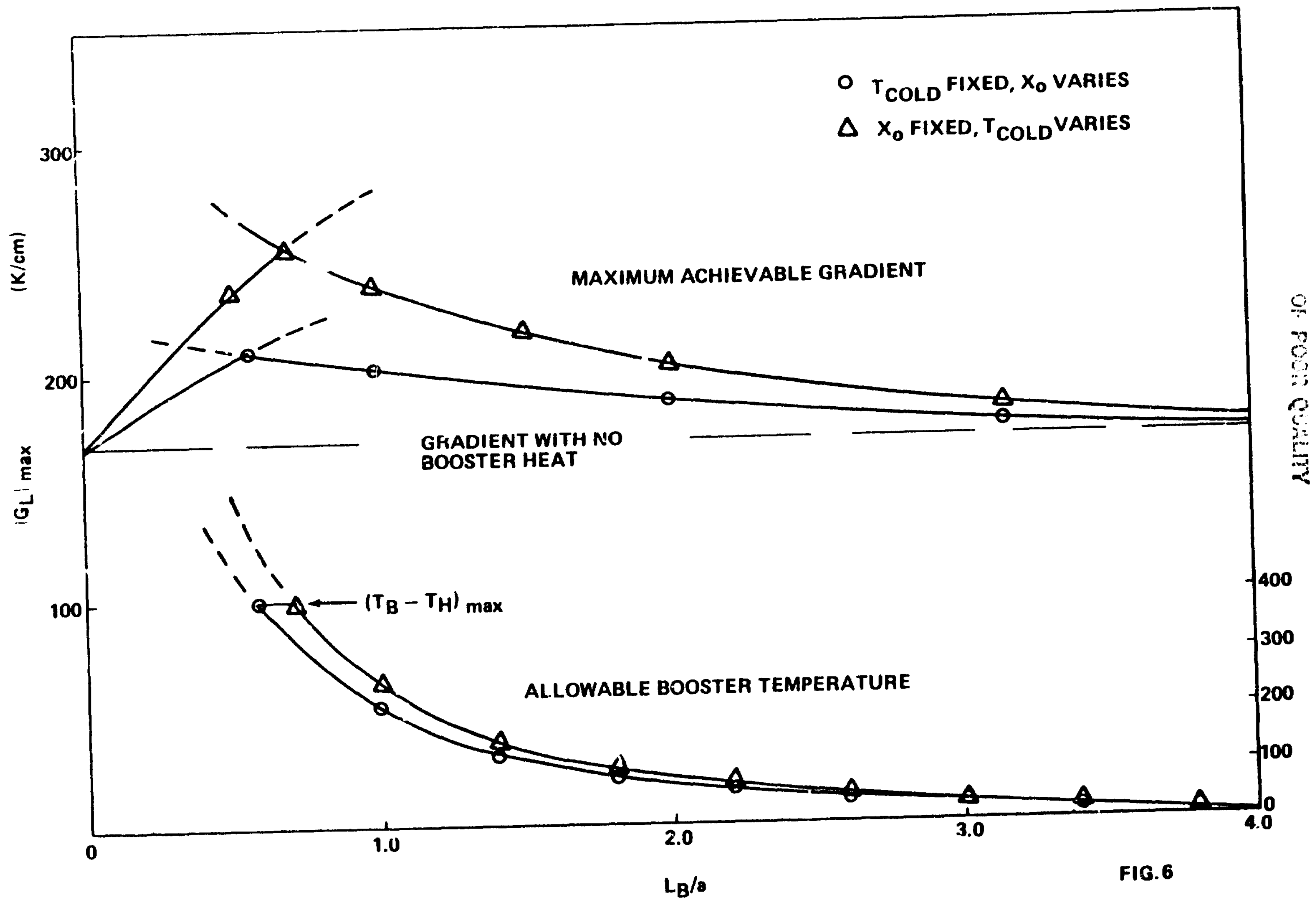

FIG. 6

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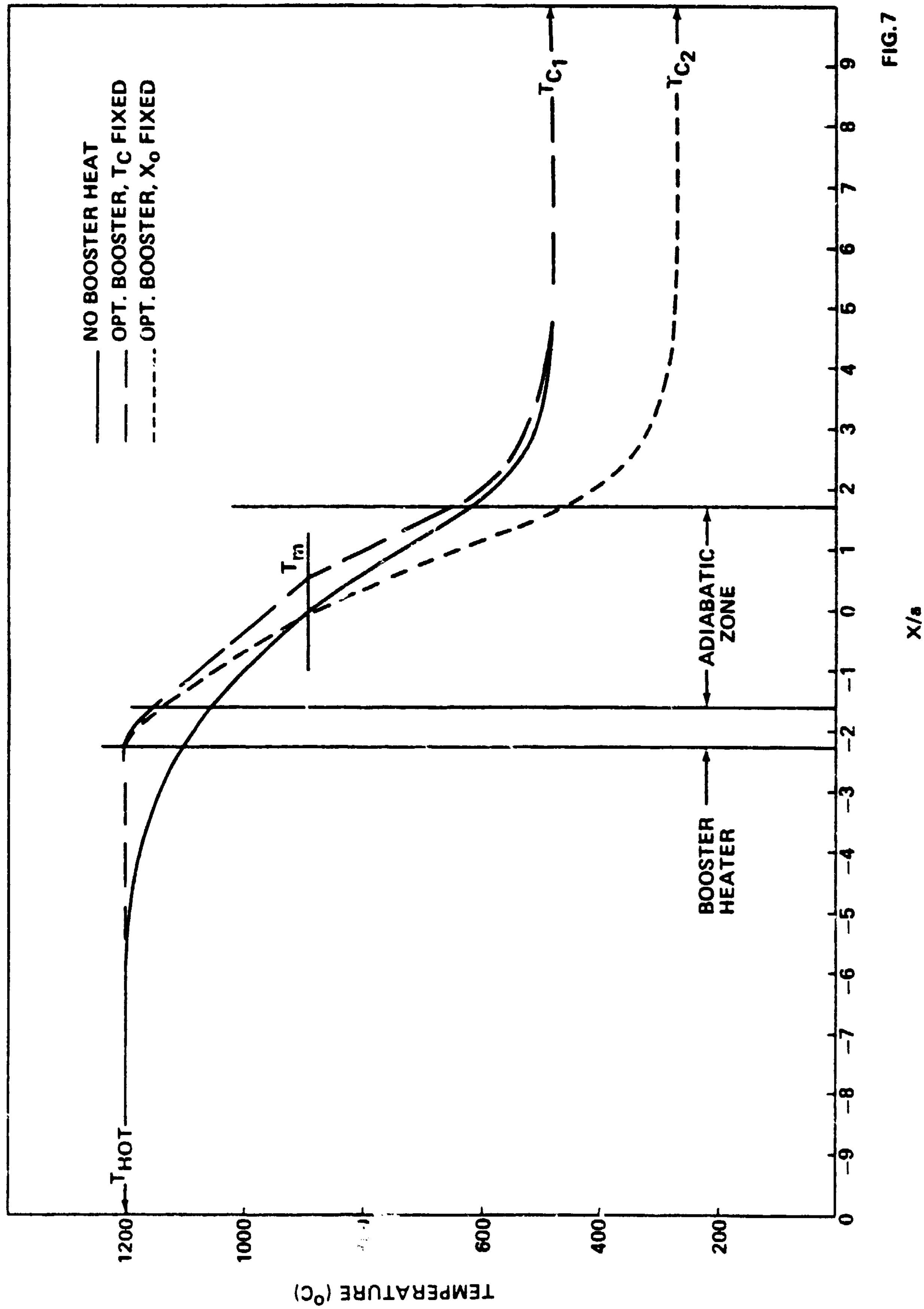

FIG.7

APPROVAL

AN ANALYTICAL APPROACH TO THERMAL MODELING OF BRIDGMAN-TYPE CRYSTAL GROWTH: ONE-DIMENSIONAL ANALYSIS

Computer Program Users Manual

By Ernestine Cothran

The information in this report has been reviewed for technical content. Review of any information concerning Department of Defense of nuclear energy activities or programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

A. J. Dessler
Director, Space Sciences Laboratory

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