report no. 81HV001
march 1981

prepared for MSFC
under contract
no. NAS8-33573

ANALYSIS AND CALCULATION OF MACROSEGREGATION IN A CASTING INGOT

volume 2 - operating guide and software documentation for the unsteady model

prepared by
the General Electric Co
huntsville operations
space systems division
huntsville alabama

GENERAL ELECTRIC

REPORT NO: 81HV001

DATE: MARCH 1981

MPS SOLIDIFICATION MODEL

VOLUME II: OPERATING GUIDE AND SOFTWARE DOCUMENTATION FOR THE UNSTEADY MODEL

PREPARED FOR

MARSHALL SPACE FLIGHT CENTER

UNDER

CONTRACT NO. NAS8-33573

PREPARED BY: Anna L. Maples

Anna L. Maples
Program Manager

APPROVED BY: L. A. Kelly

Lowell A. Kelly, Manager
Huntsville Operations

TABLE OF CONTENTS

SECTION 1
INTRODUCTION

This volume describes the operation of solidification Model 2 and it provides documentation of the software associated with the model. Model 2 calculates the macrosegregation in a rectangular ingot of a binary alloy as a result of unsteady horizontal axisymmetric bidirectional solidification. A description of the physics and numerical techniques is in Volume 1 of this report.

The solidification program allows interactive modification of calculation parameters as well as selection of graphical and tabular output. In batch mode, parameter values are input in card image form and output consists of printed tables of solidification functions. The operational aspects of Model 2 that differ substantially from Model 1 are described in Section 2. A complete guide for running Model 1 on the Prime 400 system at MSFC is in Volume III of reference 1. Section 2 assumes no familiarity with programming, but it does assume the reader is familiar with Volume 1.

Section 3 of this report contains the global flow diagrams and data structures of Model 2. As with Model 1, the primary program documentation is the code itself. It is assumed that any reader requiring the information in Section 3 thoroughly familiar with the calculation described by Volume 1, with the program operating characteristics, and with the FORTRAN language.

SECTION 2

OPERATING GUIDE

The operation of solidification Model 2 is very similar to that of Model 1. The input phase and output selection phase operate as for Model 1. The specific input parameters for Model 2 are described below. Output checkpoint control is a new procedure with Model 2; interactive checkpoint control is described in Section 2.1, and batch checkpoint control is described in Section 2.2. The mechanics of interacting with the Prime system are described in reference 1.

2.1 RUNNING THE MODEL IN INTERACTIVE MODE

The procedure for logging in to the Prime 400 system, starting the model, and running the input and output phases is the same as for Model 1 with the exception of the commands for starting Model 2. After logging in, to invoke execution of Model 2 enter the commands

```
CO MPS2
SEG #MPS2
```

Because of the time stepping nature of the unsteady model, the operation of the calculation phase is unlike the operation of Model 1. After the input phase is complete, the model takes one step away from the chill and then prints the message shown below.

```
ENTER  T TO DISPLAY TABULAR DATA,
       G TO DISPLAY GRAPHS,
       C TO CONTINUE THIS CASE,
       Q TO TERMINATE RUN, OR
       N TO PROCEED TO NEXT CASE.
C
```

This choice of action is given to the user at each checkpoint. Entering a G or a T will cause the program to go to the output phase in which the user can select specific graphical or tabular output from the calculation up to that point. When the user leaves the output phase, the selection shown above is again presented. The user can switch freely between tabular and graphical output or he can continue the calculation, start a new case or terminate execution. If the continue (C) option is selected, the program will display the following.

```
TIME SINCE BEGINNING OF SOLIDIFICATION = 0.470586     SEC.

LIQUIDUS ISOTHERM IS 0.799995E-02 CM FROM CHILL.
EUTECTIC ISOTHERM IS -1.99200     CM FROM CHILL.

ENTER EITHER THE TIME OF THE NEXT CHECKPOINT IN THE FORMAT  T=VALUE
          OR THE LIQUIDUS LOCATION AT THE NEXT CHECKPOINT IN THE FORMAT  L=VALUE
          OR THE EUTECTIC LOCATION AT THE NEXT CHECKPOINT IN THE FORMAT  E=VALUE
```

The checkpoint procedure puts the user in control of the progress of the calculation. The stopping places specified by the user as checkpoints allow him to inspect the progress of the calculation or display the current state of the S/L zone at any point in the solidification process. For convenience the stopping point may be specified by time, by eutectic front location, or by liquidus isotherm location. For example, to set up the next checkpoint at the instant when eutectic forms at the chill, enter

E=0.

To stop the model when the dendrites first reach the centerline in a mold of half-width 2 cm., enter

L=2.

To run the solidification through to completion enter a eutectic front position greater than or equal to the mold half-width.

The unsteady model allows greater flexibility in plot setup than the steady model with plot function scales brought under user control. In all cases the program will calculate a scaling and then give the user the alternative of proceeding with the calculated scaling or entering a different scale. For vector plots the scale is a single vector magnitude, for contour plots the variables are a base level value and an interval between levels, for profile plots the scale is specified as a range with a remote exponent and the number of tic intervals. If a nonzero remote exponent, say 3, is to be used the actual plot interval bounds should be multiplied by 10^3 before they are input. Profile plots over the final solid also require that the user enter the x or y location of the profile, where x is always the distance from the chill in cm., and y is the distance from the botton of the ingot in cm. Any number of profiles can be put on one plot, but the line patterns will repeat after 6. Example 4.1 shows plot scale input and profile selection.

2.2 RUNNING THE MODEL IN BATCH MODE

The batch operating procedure is the same as for Model 1 with the exception of some modifications to the input files for specification of checkpoints. The command which starts execution of the model in batch mode is

CO MPS2.BATCH

Checkpoints are defined on cards immediately following the parameter cards, one checkpoint per card. The end of the case is denoted by a card with the word END starting in column one. The checkpoint card has three fields. The first field begins in column 1 and must be one of the letters T, L or E denoting time, liquidus isotherm position or eutectic front position. The second field runs from column 6 to column 15 with the FORTRAN format E10.3. This field should contain the value specified for the checkpoint location. The third field begins in column 16 and specifies the selection of tabular output to be printed at the checkpoint. Each column controls one table, with the assignment in the same order as the interactive tabular output selection shown in example 4.1. A one in the column corresponding to a table will cause that table to be printed at the checkpoint. If the column is blank, the table will not be printed. Thus, a one in column 17 would cause the final local average composition to be printed. Any number or combination of tables may be printed at each checkpoint.

Batch cases can be stacked as before, with the case name card for case M following immediately after the END card of case M-1. A sample batch case is shown in Section 4.2.

2.3 INPUT PARAMETERS

Described below are the parameters which define a particular case of unsteady horizontal bidirectional solidification in a casting. The same set of parameters is used in both interactive and batch modes. The default case is the case that is built-in to the interactive I/O controller: The parameters take on their default values each time interactive execution is initiated. There is no default case for a batch run: all parameters must be specified for each case. The format for the batch cards is given in Section 2.2 and reference 1. Interactive parameter selection and modification is described in reference 1.

2.3.1 Alloy Specification

The binary alloy is specified by chemical symbols exactly as is done in Model 1, and Model 2 uses the same data base as Model 1. The default alloy is Al-4.5%Cu.

2.3.2 Solidification Process Parameters

The parameters in this group describe the conditions under which the casting is made including the mold geometry, the thermal conditions, and the strength of the gravitational force.

Parameter Description	Symbol	Default	Limits
Mold half width	x_c	2.7 cm	$x_c>0$
Mold height	L	6.35 cm	$L>0$
Isotherm time exponent	q	1	$q>0$
Liquidus coefficient	b_L	.017 cm/sec	$b_L>0$
Eutectic coefficient	b_E	.017 cm/sec	$b_E>0$
Initial separation	a_E	-2. cm	$a_E<0$
Gravitational force in -y direction	g	1G	$g\geq0$

As noted in Section 3.2.2 of Volume I, the unsteady model is limited to cases in which the temperature of the chill is brought below the eutectic temperature gradually rather than instantaneously. This restriction implies a_E must be significantly less than the upper limit shown above. Results for cases with a_E close to zero are not predictable.

2.3.3 Permeability

The permeability model in the unsteady model is identical to that in the steady-state model. The default value of γ is $6X10^{-7}$ cm^2.

2.3.4 Numerical Methods Control Parameters

In the majority of cases the parameters in this group should not be changed from their default values, however operator control of these parameters could be useful in trouble-shooting. The parameters are explained in the discussions of numerical methods in Volume 1 of this report and Volume I of reference 1.

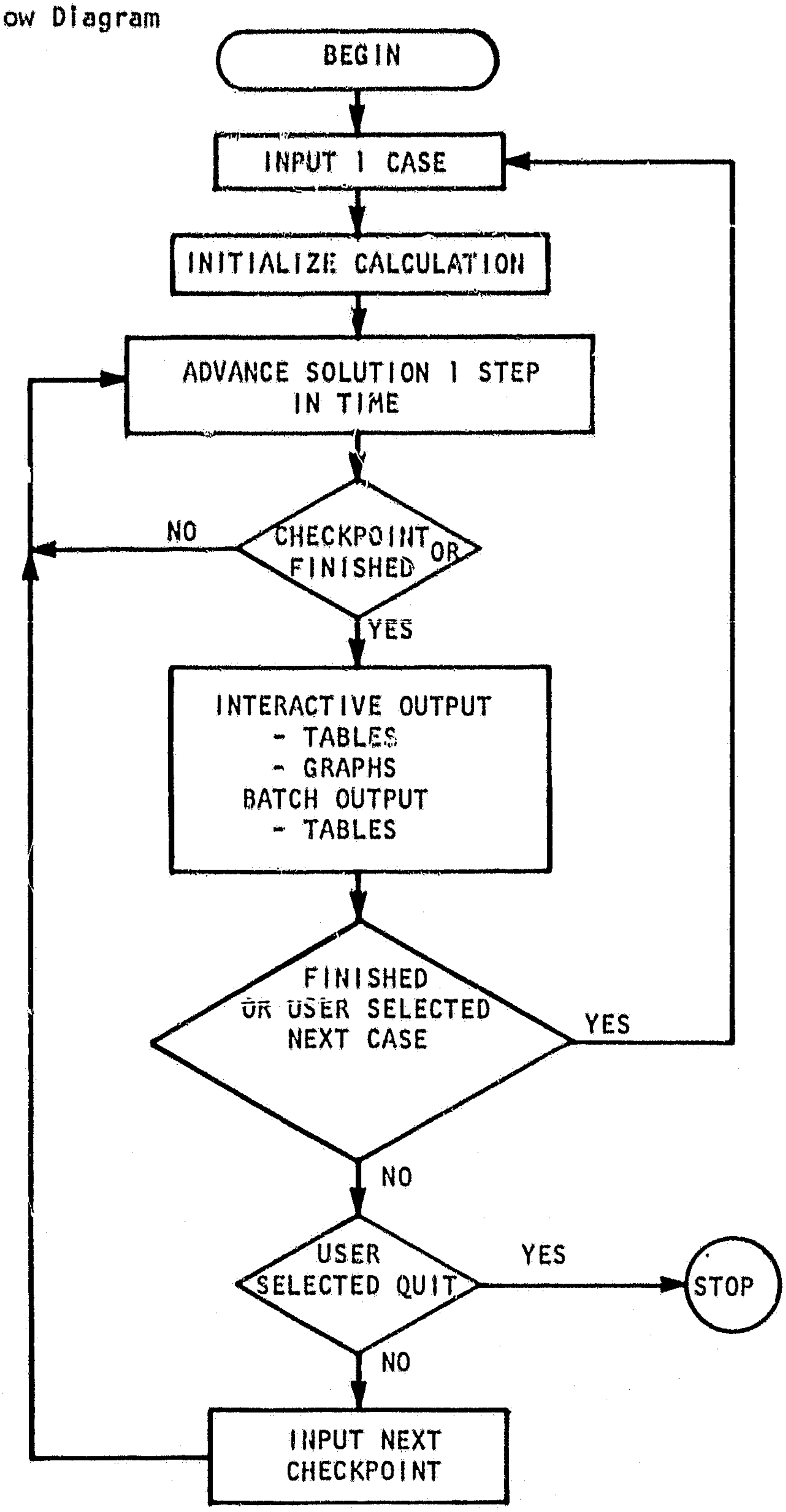
Parameter Description	Symbol	Default	Limits
Number of horizontal mesh points	N_I	20	$4 \le N_I \le 50$
Number of vertical mesh points	N_J	10	$3 \le N_J \le 50$
Maximum number of pressure iterations	M_{SOR}	200	$M_{SOR} > 0$
Pressure convergence criterion	E_{SOR}	10^{-4}	$E_{SOR} > 5X10^{-6}$
Fraction of CFL step to take	f	.5	$0 < f < 1$
Maximum step size in x_E	Δx_E	.1 cm	$\Delta x_E > 0$
Initial g_L at chill	g_{LI}	.9	$.1 < g_{LI} < 1.$
Minimum horizontal mesh size	N_{Imin}	4	$4 \le N_{Imin} \le 50$

SECTION 3

PROGRAMMERS GUIDE

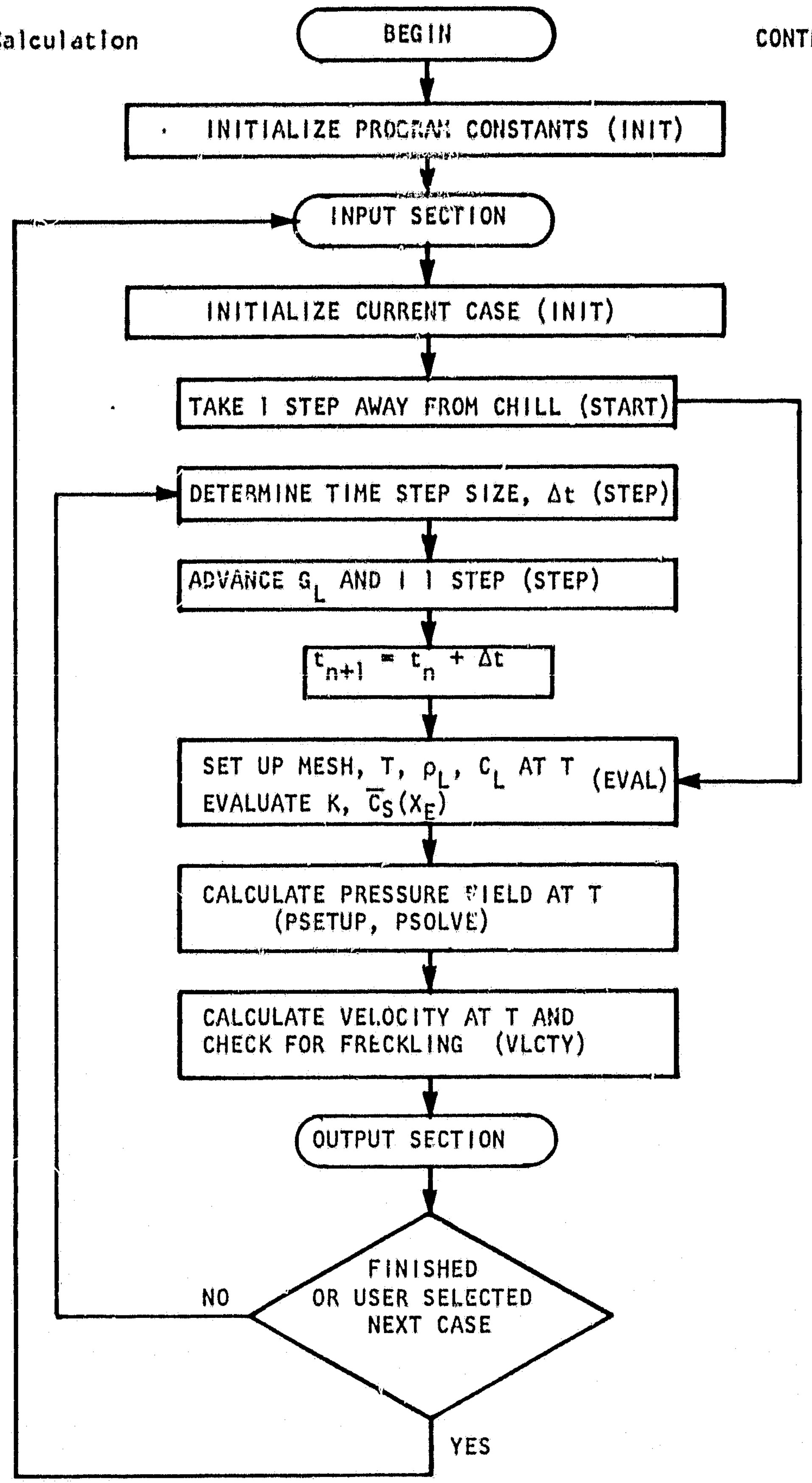
3.1 FLOW DIAGRAMS

3.1.1 Global Flow Diagram

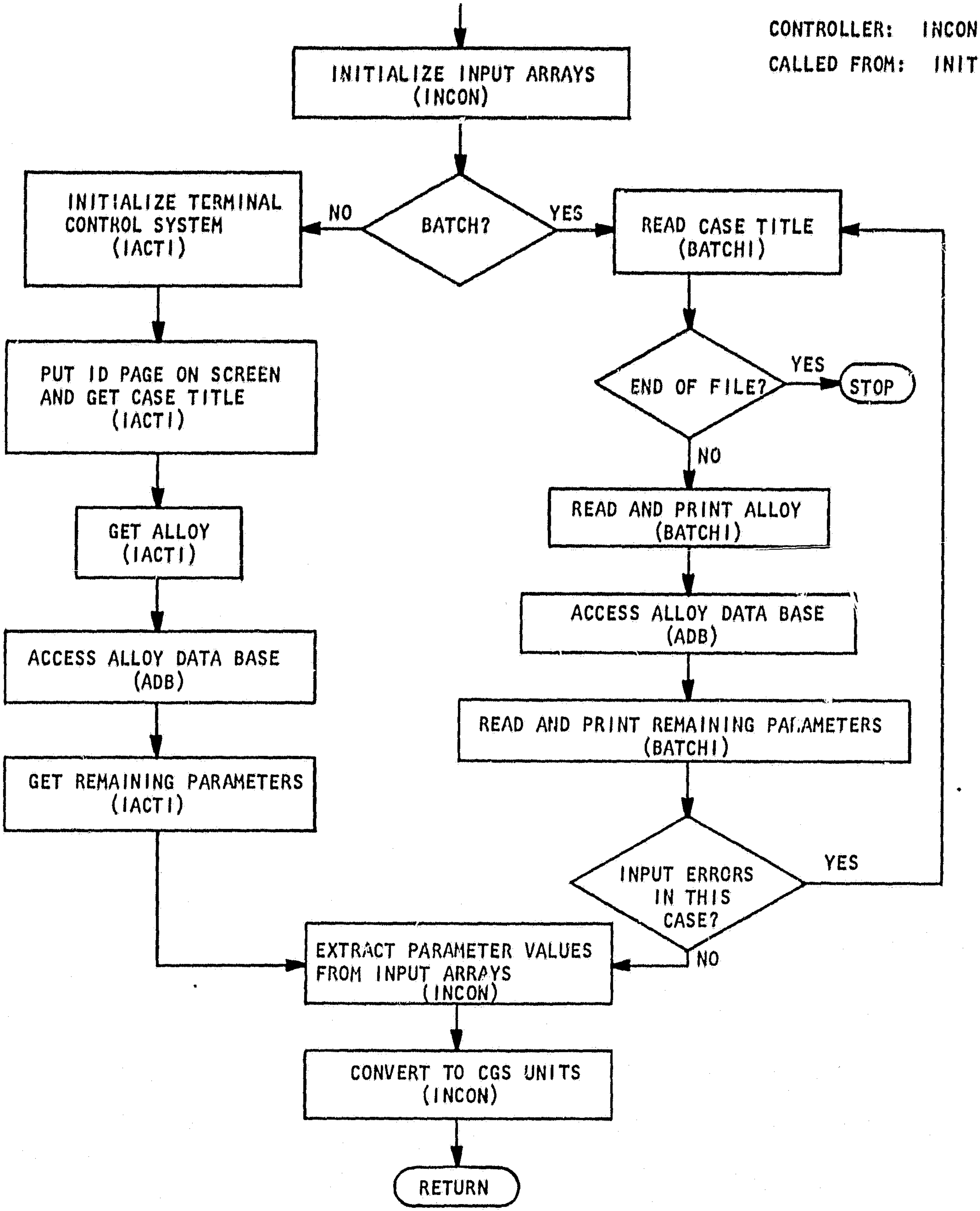


3.1.2 Calculation

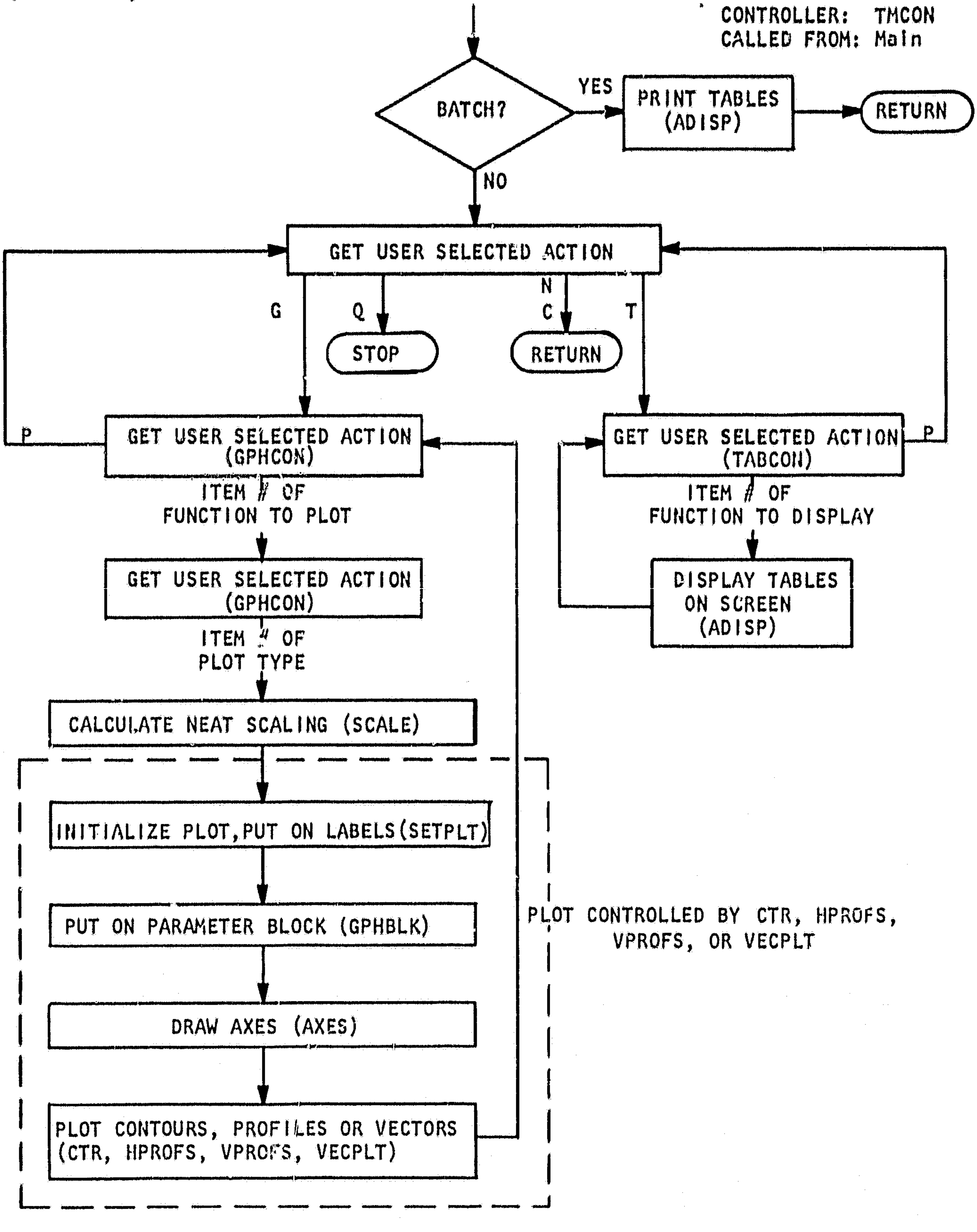
CONTROLLER: MAIN



3.1.3 Input Section



3.1.4 Output Section



3.2 ALPHABETICAL LIST OF SUBROUTINES

The list below contains only the modules that were written specifically for the solidification model. Off-the-shelf routines used by the model are listed in Sections 3.2 and 3.3 of reference 1. The purpose of each routine is described briefly below; details of the programming, including calling sequence descriptions, are in the program comments.

NAME	SECTION	FUNCTION
ADB	I/O	Retrieve phase diagram, densities and viscosity from alloy data base.
ADISP	I/O	Displays any array on the screen or in printed form.
ALNUIN	I/O	Gets interactive input that may be either alphanumeric or numerical.
AXES	Graphics	Draws and labels axes on all plots.
BATCHI	I/O	Controls batch mode card input.
COORD	Calculation	Calculates isotherm positions and coordinate transformation.
CTR	Graphics	Controls contour plots.
CTRBOX	Graphics	Logic for contouring over given rectangular region.
CTRDRW	Graphics	Draws contour line elements.
CTRLAB	Graphics	Labels contour level values.
DISKC	I/O	Performs various control functions on disk files.
DISKI	I/O	Retrieves final solid data from temporary disk for use by graphics routines.
DISKO	I/O	Writes final solid data on temporary disk.
EVAL	Calculation	Evaluates specified functions at current time.
GPBLK	Graphics	Puts parameter block on plot.
GPHCON	Graphics	Controls interactive graphics.
GRIDCN	Calculation	Controls size of computational grid.
GRIDXE	Calculation	Sets up computational grid.
HPROFS	Graphics	Controls horizontal profile plots.
IACTI	I/O	Controls interactive input.
INCON	I/O	Controls input section.
INIT	Calculation	Initialization routine.
MASSCK	I/O	Monitors conservation of mass.
MSG	I/O	Puts any brief message on terminal screen.

NAME	SECTION	FUNCTION
PERM	Calculation	Calculates permeability.
PSETUP	Calculation	Calculates $\vec{A}$, and B and sets up boundary conditions (see equations 1.3.4.4 to 1.3.4.11)
PSOLVE	Calculation	Solves the pressure equation (see reference 1, Vol. 1, 4.5)
SCALE	I/O	Calculates neat scales for plots.
SETHOL	I/O	Sets up long hollerith arrays.
SETPLT	Output	Initializes all plots and puts on labels.
START	Calculation	Takes first step away from chill. (See Vol. 1, Section 4.3)
STEP	Calculation	Advances g_L and I one step (See Vol 1, Section 4.4)
TABCON	I/O	Controls tabular output
TMCON	I/O	Controls display checkpoints and time-varying I/O.
VECPLT	Output	Controls plots of vector fields.
VLCTY	Calculation	Calculates velocity.
VPROFS	Output	Controls vertical profile plots.
WAIT	Output	Waits for the operator to enter a P.

3.3 KEY PROGRAM SYMBOLS

A description of all common block items is at the end of subroutine INIT.

PROGRAM SYMBOL	COMMON BLOCK	DEFINITION (See Volume 1, Section 2)
AE	/PROCSS/	a_E
AGC	/SLZONE/	I
ALNAM	/ALLOY/	Element 1 is the hollerith solvent name. Element 2 is the hollerith solute name.
BE, BL	/PROCSS/	b_E, b_L
CL	/SLZONE/	C_L
CLØ	/ALLOY/	C_o
DCLDT	/ALLOY/	dC_L/dT
DRHDC	/ALLOY/	$d\rho_L/dC_L$
DTDTM	/SLZONE/	$\partial T/\partial t = \varepsilon$
DTM	/MESH/	Δt
DXI	/MESH/	$\Delta \xi$
DET	/MESH/	$\Delta \eta$
EPR	/ALLOY/	k

PROGRAM SYMBOL	COMMON BLOCK	DEFINITION (See Volume 1, Section 2)
ET	/MESH/	η
FLAC	/SLZONE/	$\overline{C}_S(x_E)$
GAMMA	/PMBLTY/	γ
GL	/SLZONE/	g_L
GMY	/PROCSS/	g
HMOLD	/PROCSS/	ℓ
KK	/PMBLTY/	K
NI	/MESH/	N_i
NJ	/MESH/	N_j
P	/SLZONE/	p
QLE	/PROCSS/	q
RHL	/SLZONE/	ρ_L
RHLE	/ALLOY/	ρ_{LE}
RHS	/ALLOY/	ρ_S
RHSE	/ALLOY/	ρ_{SE}
T	/SLZONE/	T
TE	/ALLOY/	T_E
TM	/MESH/	t
V	/SLZONE/	$\vec{V}$
WMOLD	/PROCSS/	x_C
X	/MESH/	x
Y	/MESH/	y
XE, XL	/PROCSS/	x_E, x_L
XI	/MESH/	ξ

3.4 PROGRAM CONFIGURATION ON THE PRIME

The procedures described in this section are used to maintain the program on the Prime 400 system.

3.4.1 Compilation

If the FORTRAN source code is stored in a file named MPS2.PGM, then it can be compiled by entering the command

```
FTN MPS2.PGM 2/500
```

3.4.2 Linking

The Prime utility for linking and running segmented programs in SEG. It can be used to build a run file as follows:

```
SEG
LO #MPS2
LO B_MPS2.PGM
LIB VAPPLB
LIB TCS500
LIB
SAV
Q
```

3.5 EXECUTION COMMAND FILES

After the run file #MPS2 has been built, the program can be executed by entering the commands described in Section 2. The execution is set up and controlled by two command files listed below:

Command File MPS2	Command File MPS2.BATCH
OPEN ICARD 1 1	OPEN CARDS 1 1
CO -END	SEG #MPS2
	C 1 2 3
	CO -END

CARDS is a disk file containing the batch card input, and ICARD contains the single word INTERACTIVE. CARDS or ICARD is accessed by the program via FORTRAN logical unit number 5. Other files used by the program are M1.D.B, the data base file; DISK, the temporary disk storage file; and PRINT the batch printed output file. M1.D.B is accessed via logical unit number 7, DISK is on logical unit number 8, and PRINT is on logical unit 6. No printed output is generated by an interactive mode run.

SECTION 4
SAMPLE CASES

4.1 INTERACTIVE CASE

The case shown here is the Al-4.5% Cu case that the interactive model will run if none of the input parameters are changed from their default values. This case demonstrates the use of the checkpoint control to run the case through completion, and several output options that are new with the unsteady model. Any of the non-vector functions can be displayed on a contour plot, the one shown is contours of final composition over the entire ingot. Note that the location of the function maximum and minimum are marked on the plot by an x and an o. The base level, $\overline{C}_S$ = 4.5% Cu in this case, is drawn with a heavy line. Levels below the base level are drawn with dashed lines and those above are drawn with solid lines. Every fifth level is drawn with a heavy line. The selection of the base level and the interval between levels is under user control as shown on the plot selection page preceeding the sample contour plot. The next plot is horizontal profiles of final composition, using the default scaling showing the selection of three profiles. The last plot is vertical profiles of final composition, illustrating the change in plot scale. In addition to the plots shown here, all plots that were available in the steady-state model are also available in the unsteady model. The final output for this case is the tabular display of the metal mass balance and the solute mass balance at the end of solidification.

```
MATERIALS PROCESSING IN SPACE

MACROSEGREGATION IN A CASTING INGOT

MODEL  B
 1 UNIDIRECTIONAL SOLIDIFICATION OF A BINARY ALLOY
 1 UNSTEADY SOLUTION
 1 PLANAR ISOTHERMS, RECTANGULAR MUSHY ZONE
 1 ISOTHERM MOVEMENT INPUT
 1 TEMPERATURE GRADIENT ASSUMED
 1 NO CONVECTION IN BULK LIQUID
 1 ISOTROPIC PERMEABILITY K= GAMMA*GL**8


ENTER CASE TITLE (UP TO 80 CHARACTERS)
................................................................................
```

```
ALLOY

     SOLVENT:  AL
     SOLUTE:   CU    WEIGHT PERCENT: 4.500E 00

ENTER A TO CHANGE ALLOY OR      P TO PROCEED.
P
```

```
ALLOY DATA BASE  -  DATA BASE REVISED 4/30/80

SOURCE OF INFORMATION FOR  AL  -CU       0.000E-01 TO  3.300E 01 WT. PCT. CU
   PHASE DIAGRAM - M.C. FLEMINGS AND G. NEREO, MET TRANS, VOL 239, 1967, P 1449.
   DENSITIES     - R. MEHRABIAN, M. KEANE AND M.C. FLEMINGS, TRANS TMS-AIME,
                   VOL 1, 1970, P 1209.
   VISCOSITY     - R. MEHRABIAN, M. KEANE AND M.C. FLEMINGS, TRANS TMS-AIME,
                   VOL 1, 1970, P 1209.

PHASE DIAGRAM
   TEMPERATURE-COMPOSITION SLOPE                 -2.880E-01 PCT SOLUTE / DEG C
   EQUILIBRIUM PARTITION RATIO                    1.720E-01
   EUTECTIC COMPOSITION                           3.300E 01 PCT SOLUTE
   EUTECTIC TEMPERATURE                           5.480E 02 DEG C

DENSITIES
   COMPOSITION-DENSITY SLOPE                      2.670E-02 (GM/CM**3) / PCT SOLUTE
   SOLID DENSITY                                  2.620E 00 GM/CM**3
   LIQUID EUTECTIC DENSITY                        3.220E 00 GM/CM**3
   SOLID EUTECTIC DENSITY                         3.400E 00 GM/CM**3

VISCOSITY                                         3.000E-02 GM/(CM*SEC)


ENTER P TO PROCEED
P
```

```
AL    4.5000    CU      SOLIDIFICATION MODEL  2     09:09:02    THU, JAN 29 1981


SOLIDIFICATION PROCESS PARAMETERS
 1     MOLD (HALF) WIDTH                          2.700E 00     (CM)
 2     MOLD HEIGHT                                6.350E 00     (CM)
 3     ISOTHERM TIME EXPONENT (Q)                 1.000E 00
 4     LIQUIDUS ISOTHERM COEFFICIENT (BL)         1.700E-02     (CM/SEC)
 5     EUTECTIC ISOTHERM COEFFICIENT (BE)         1.700E-02     (CM/SEC)
 6     INITIAL ISOTHERM SEPARATION (AE)          -2.000E 00     (CM)
 7     GRAVITATIONAL FORCE                        1.000E 00     (G)


ENTER ITEM NUMBER TO CHANGE, OR
      P            TO PROCEED.
P
```

```
AL    4.5000    CU      SOLIDIFICATION MODEL  2     09:09:02    THU, JAN 29 1981


PERMEABILITY MODEL PARAMETERS
 1     GAMMA                                      6.000E-07     (CM**2)


ENTER ITEM NUMBER TO CHANGE, OR
      P            TO PROCEED.
```

```
AL    4.5000    CU      SOLIDIFICATION MODEL  2     09:09:02    THU, JAN 29 1981


NUMERICAL METHODS CONTROL PARAMETERS
 1     NUMBER OF HORIZONTAL MESH POINTS                  20
 2     NUMBER OF VERTICAL MESH POINTS                    10
 3     MAXIMUM NUMBER OF PRESSURE ITERATIONS            200
 4     PRESSURE CONVERGENCE CRITERION             1.000E-04
 5     FRACTION OF CFL STEP TO TAKE               5.000E-01
 6     MAXIMUM STEP SIZE IN XE                    1.000E-01     (CM)
 7     INITIAL VOLUME FRACTION LIQUID AT CHILL    9.000E-01
 8     MINIMUM HORIZONTAL MESH SIZE                       4


ENTER ITEM NUMBER TO CHANGE, OR
      P            TO PROCEED.
P
```

CALCULATION IN PROGRESS FOR CASE

AL 4.5000 CU SOLIDIFICATION MODEL 2 00:00:02 THU, JAN 29 1981

TIME	STEP SIZE	PRESSURE CYCLES	XE	XL
1.88234	0.000000	11	-1.96800	0.319998E-01

ENTER T TO DISPLAY TABULAR DATA,
G TO DISPLAY GRAPHS,
C TO CONTINUE THIS CASE,
Q TO TERMINATE RUN, OR
N TO PROCEED TO NEXT CASE.

C

TIME SINCE BEGINNING OF SOLIDIFICATION = 1.88234 SEC.

LIQUIDUS ISOTHERM IS 0.319998E-01 CM FROM CHILL.
EUTECTIC ISOTHERM IS -1.96800 CM FROM CHILL.

ENTER EITHER THE TIME OF THE NEXT CHECKPOINT IN THE FORMAT T=VALUE
OR THE LIQUIDUS LOCATION AT THE NEXT CHECKPOINT IN THE FORMAT L=VALUE
OR THE EUTECTIC LOCATION AT THE NEXT CHECKPOINT IN THE FORMAT E=VALUE

E=2.7

NEXT CHECKPOINT WILL BE AT T = 276.470 SEC., XL = 4.69998 CM., XE = 2.69998 CM.

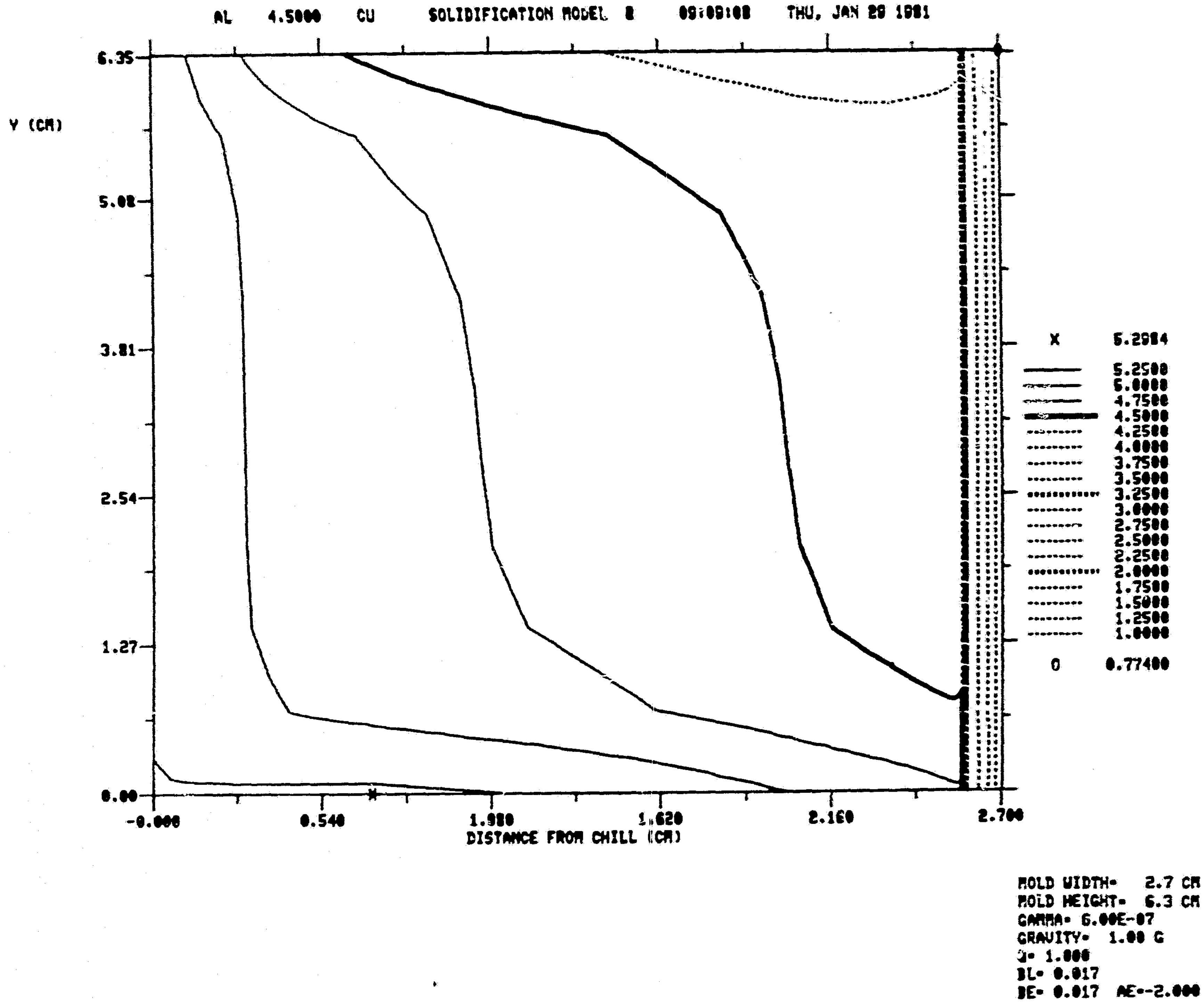
TIME	STEP SIZE	PRESSURE CYCLES	XE	XL
2.82351	0.941170	10	-1.95200	0.479997E-01
4.23527	1.41176	17	-1.92800	0.719996E-01
5.29408	1.05882	15	-1.91000	0.[illegible]99993E-01
6.61760	1.32352	14	-1.88750	0.118499
8.27200	1.65440	23	-1.85938	0.140884
9.65066	1.37867	22	-1.83594	0.164061
11.2591	1.60844	21	-1.80860	0.191405
13.1356	1.87652	25	-1.77669	0.223305
14.7776	1.64195	26	-1.74878	0.251818
⋮	⋮	⋮	⋮	⋮
245.521	2.01039	22	2.17385	4.17385
247.381	1.85958	22	2.20546	4.20647
249.101	1.71989	27	2.23470	4.23470
250.958	1.85784	22	2.26688	4.26688
252.653	1.69482	22	2.29610	4.29610
254.199	1.54596	24	2.32138	4.32138
255.894	1.69484	25	2.35019	4.35019
257.410	1.51577	26	2.37695	4.37696
258.765	1.35549	21	2.39900	4.39900
260.284	1.51878	22	2.42428	4.42428
261.601	1.31729	22	2.44781	4.44781
262.744	1.14233	14	2.46663	4.46663
264.070	1.32634	15	2.48918	4.48918
265.160	1.09010	16	2.50770	4.50770
266.056	0.895791	9	2.52894	4.52894
267.169	1.11380	10	2.54187	4.54187
267.982	0.812863	10	2.55569	4.55569
268.575	0.592910	10	2.56577	4.56677
269.008	0.432339	10	2.57311	4.57311

SOLIDIFICATION COMPLETE.

ENTER T TO DISPLAY TABULAR DATA,
G TO DISPLAY GRAPHS,
Q TO TERMINATE RUN, OR
N TO PROCEED TO NEXT CASE.

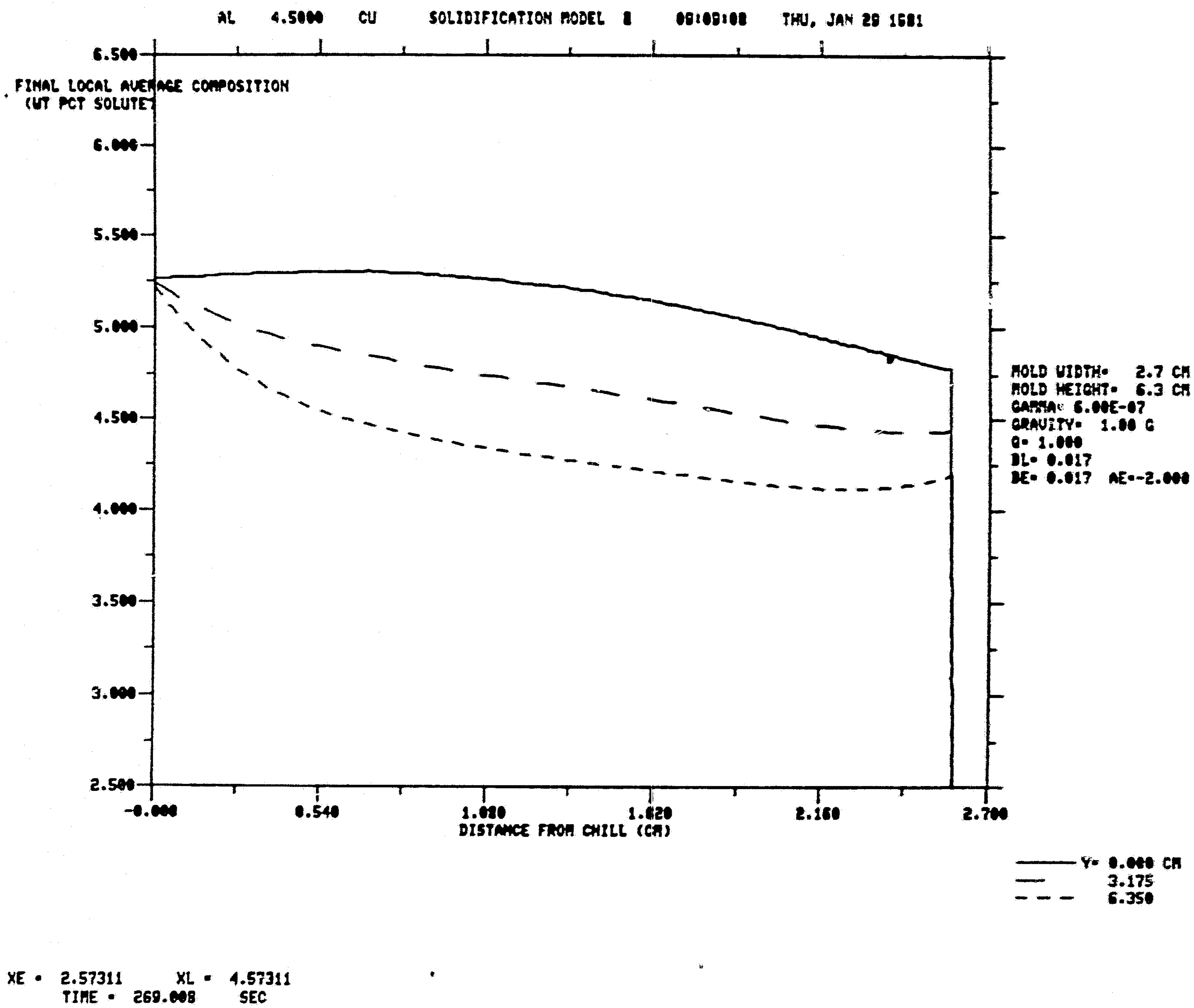
G

```
AL    4.5000    CU      SOLIDIFICATION MODEL  2     03:09:08    THU, JAN 29 1981


     FUNCTION TO PLOT                                          PLOT TYPE

**********       S/L ZONE       **********                    1  VERTICAL PROFILES
   1  VELOCITY                                                2  HORIZONTAL PROFILES
   2  PRESSURE: P-P0                                          3  VECTOR FIELD
   3  PRESSURE - BULK HYDROSTATIC P                           4  CONTOURS
   4  FRACTION LIQUID
   5  MASS FLOW
   6  SOLUTE FLOW

**********         INGOT        **********
   7  FINAL LOCAL AVERAGE COMPOSITION
   8  VOLUME FRACTION EUTECTIC


ENTER ITEM NUMBER OF FUNCTION TO PLOT, OR
      P TO PROCEED.
7

ENTER ITEM NUMBER OF PLOT TYPE
4

FUNCTION MINIMUM = 0.774    FUNCTION MAXIMUM =  5.30

THERE WILL BE   8 LEVELS SPACED AT INTERVALS 0.500000     ABOUT A BASE LEVEL OF   4.50000

ENTER P TO PROCEED WITH THESE LEVELS, OR
      C TO CHANGE LEVELS
C


ENTER BASE LEVEL
4.5

ENTER LEVEL INTERVAL
.25


FUNCTION MINIMUM = 0.774    FUNCTION MAXIMUM =  5.30

THERE WILL BE  17 LEVELS SPACED AT INTERVALS 0.250000     ABOUT A BASE LEVEL OF   4.50000

ENTER P TO PROCEED WITH THESE LEVELS, OR
      C TO CHANGE LEVELS
P
```



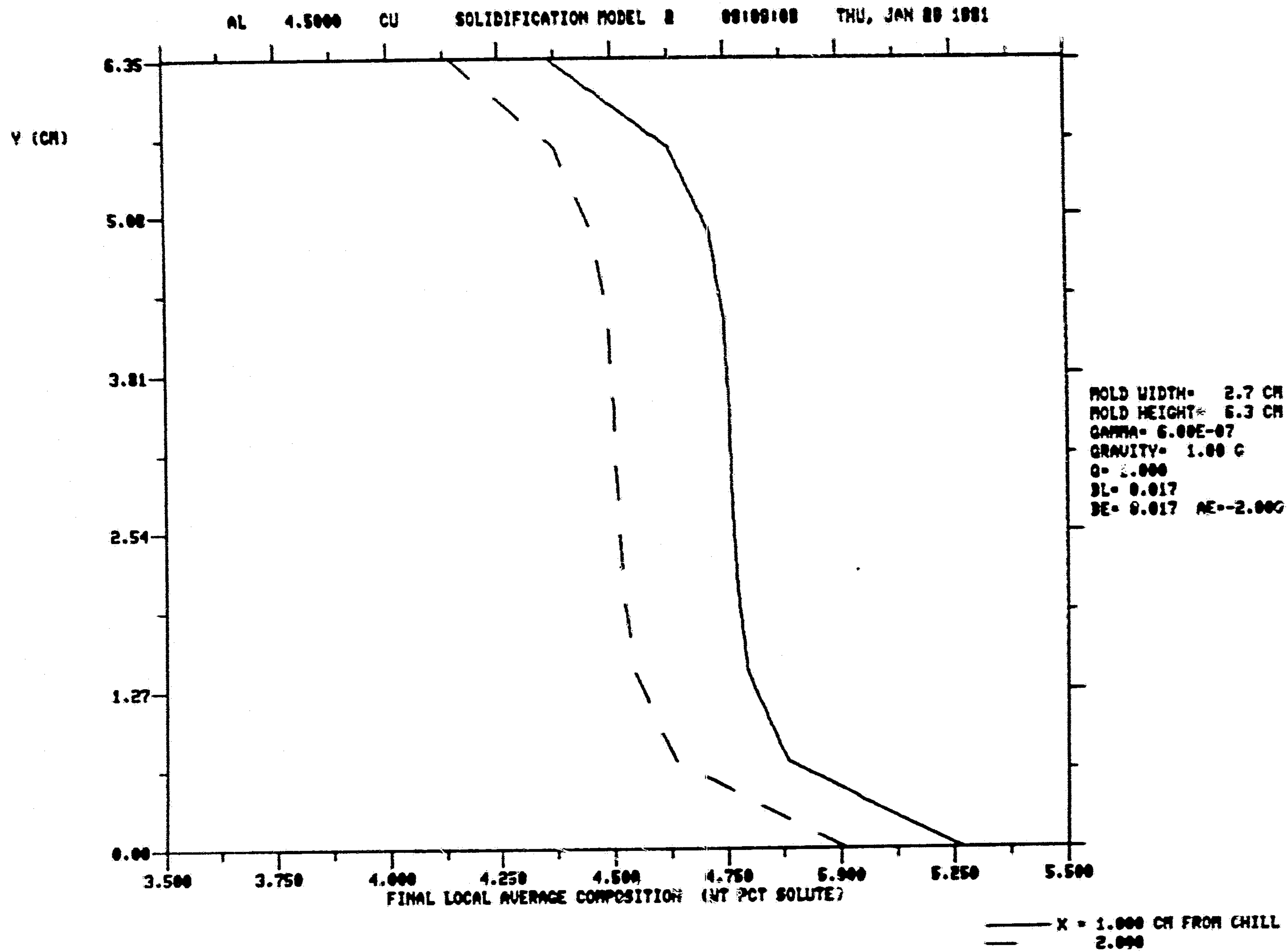
FINAL LOCAL AVERAGE COMPOSITION

```
AL    4.5000    CU      SOLIDIFICATION MODEL  2     08:09:02    THU, JAN 29 1981


     FUNCTION TO PLOT                                       PLOT TYPE

**********      S/L ZONE      **********                   1  VERTICAL PROFILES
   1  VELOCITY                                             2  HORIZONTAL PROFILES
   2  PRESSURE: P-P0                                       3  VECTOR FIELD
   3  PRESSURE - BULK HYDROSTATIC P                        4  CONTOURS
   4  FRACTION LIQUID
   5  MASS FLOW
   6  SOLUTE FLOW

**********       INGOT        **********
   7  FINAL LOCAL AVERAGE COMPOSITION
   8  VOLUME FRACTION EUTECTIC


ENTER ITEM NUMBER OF FUNCTION TO PLOT, OR
      P TO PROCEED.
7

ENTER ITEM NUMBER OF PLOT TYPE
2


MINIMUM FUNCTION VALUE IS 0.774000
MAXIMUM FUNCTION VALUE IS  5.29838


AUTOMATIC SCALING YIELDS PLOT RANGE:    2.500 TO   6.500  WITH REMOTE EXPONENT    0
OVER  8 MAJOR TIC INTERVALS


ENTER P TO PROCEED WITH AUTOMATIC SCALING, OR
      LOWER BOUND OF PLOT INTERVAL.
P


ENTER Y VALUE OF PROFILE OR      P TO PROCEED.
0


ENTER Y VALUE OF PROFILE OR      P TO PROCEED.
3.175


ENTER Y VALUE OF PROFILE OR      P TO PROCEED.
6.35


ENTER Y VALUE OF PROFILE OR      P TO PROCEED.
P
```



AL 4.5000 CU SOLIDIFICATION MODEL
THU, JAN 29 1981
FINAL LOCAL AVERAGE COMPOSITION
(WT PCT SOLUTE)
6.500
6.000
5.500
5.000
4.500
4.000
3.500
3.000
2.500
-0.000
0.540
1.080
1.620
2.160
2.700
DISTANCE FROM CHILL (CM)
MOLD WIDTH= 2.7 CM
MOLD HEIGHT= 6.3 CM
GAMMA= 6.00E-07
GRAVITY= 1.00 G
Q= 1.000
BL= 0.017
BE= 0.017 AE=-2.000
Y= 0.000 CM
3.175
6.350
XE = 2.57311 XL = 4.57311
TIME = 269.008 SEC

```
AL    4.5W/O    CU      SOLIDIFICATION MODEL  2     08:09:08    THU, JAN 29 1981

     FUNCTION TO PLOT                                       PLOT TYPE

**********      S/L ZONE      **********              1  VERTICAL PROFILES
  1  VELOCITY                                         2  HORIZONTAL PROFILES
  2  PRESSURE: P-P0                                   3  VECTOR FIELD
  3  PRESSURE - BULK HYDROSTATIC P                    4  CONTOURS
  4  FRACTION LIQUID
  5  MASS FLOW
  6  SOLUTE FLOW

**********        INGOT       **********
  7  FINAL LOCAL AVERAGE COMPOSITION
  8  VOLUME FRACTION EUTECTIC


ENTER ITEM NUMBER OF FUNCTION TO PLOT, OR
     P TO PROCEED.
7

ENTER ITEM NUMBER OF PLOT TYPE
1


MINIMUM FUNCTION VALUE IS 0.774000
MAXIMUM FUNCTION VALUE IS  5.29838

AUTOMATIC SCALING YIELDS PLOT RANGE:    2.500 TO   6.500  WITH REMOTE EXPONENT    0
OVER  8 MAJOR TIC INTERVALS

ENTER P TO PROCEED WITH AUTOMATIC SCALING, OR
      LOWER BOUND OF PLOT INTERVAL.
3.5

ENTER UPPER BOUND OF PLOT INTERVAL.
5.5

ENTER REMOTE EXPONENT
0

ENTER NUMBER OF MAJOR TIC INTERVALS.
8

FINAL SOLID FORMED BETWEEN X =-0.108741E-04 AND X =  2.70000     CM. FROM CHILL.

ENTER X VALUE OF PROFILE OR      P TO PROCEED.
1

ENTER X VALUE OF PROFILE OR      P TO PROCEED.
2

ENTER X VALUE OF PROFILE OR      P TO PROCEED.
```



XE = 2.57311 XL = 4.57311
TIME = 269.008 SEC

```
ENTER  T TO DISPLAY TABULAR DATA,
       G TO DISPLAY GRAPHS,
       Q TO TERMINATE RUN, OR
       N TO PROCEED TO NEXT CASE.
T
```

```
AL    4.5000    CU      SOLIDIFICATION MODEL  2     09:09:08    THU, JAN 29 1981


  1  MASS BALANCE TABLES
  2  FINAL LOCAL AVERAGE COMPOSITION
  3  FRACTION EUTECTIC
  4  VOLUME FRACTION LIQUID
  5  LOCAL AVERAGE SOLID COMPOSITION
  6  VELOCITY
  7  PRESSURE (P-P0)
  8  PRESSURE - BULK HYDROSTATIC P
  9  TEMPERATURE
 10  LIQUID COMPOSITION
 11  LIQUID DENSITY
 12  PRESSURE EQUATION COEFFICIENTS


ENTER ITEM NUMBER OF TABLE TO DISPLAY, OR
      P TO PROCEED.
1
```

AL 4.5000 CU SOLIDIFICATION MODEL 2 08:28:08 WED, DEC 24 1980

MASS BALANCE AT TIME = 800.000 SEC.
XL = 4.57311 CM.
XE = 2.57311 CM.

	METAL MASS (GM)	SOLUTE MASS (GM)	AVERAGE PERCENT SOLUTE
CURRENT FINAL SOLID	45.3306	2.10074	4.63336
CUMULATIVE FLOW THROUGH LIQUIDUS ISOTHERM	45.7374	2.05880	4.50004
- CURRENT S/L ZONE CONTENTS			
CURRENT S/L ZONE CONTENTS	0.000000	0.000000	0.000000
PREVIOUS S/L ZONE CONTENTS	-0.161755E-02	-0.457020E-03	30.1085
+ FLOW IN THROUGH LIQUIDUS ISOTHERM			
- FLOW OUT THROUGH EUTECTIC ISOTHERM			
CURRENT BULK MELT CONTENTS	0.000000	0.000000	0.000000
INITIAL MOLD CONTENTS	-3.57698	-0.160984	4.50054
- CUMULATIVE FLOW THROUGH LIQUIDUS			
CURRENT MOLD CONTENTS	45.3306	2.10074	4.63336
INITIAL MOLD CONTENTS	42.1604	1.89722	4.50000

ORIGINAL PAGE IS
OF POOR QUALITY

4.2 BATCH CASE

This example shows the same Al-4.5%Cu case as example 4.1, except it is for zero gravity and it is run in batch mode. Note that output is at checkpoints only and only of current function values. This, to get a table of final composition across the ingot the user must set up a checkpoint card at each value of x_E where data is required. The deck used to run this case is shown below. In this there are three checkpoints. At the first final composition and volume fraction solid across the S/L zone when $x_E = 0$ (chill face) are selected by putting one's in columns 17 and 19. At the second only final composition is printed, and at the third final composition and fraction eutectic are printed.

```
BATCH
BATCH EXAMPLE
AL
CU
4.5
2.7                                MOLD HALF WIDTH (CM)
6.35                               MOLD HEIGHT (CM)
1.                                 Q
.017                               BL
.017                               BE
-2.                                AE
0.                                 GRAVITY (G)
6.E-7                              GAMMA (CM**2)
20                                 NUMBER OF HORIZONTAL MESH POINTS
3                                  NUMBER OF VERTICAL MESH POINTS
200                                MAXIMUM NUMBER OF PRESSURE ITERATIONS
1.E-4                              PRESSURE CONVERGENCE BOUND
.5                                 FRACTION OF CFL STEP
.1                                 MAXIMUM STEP IN XE
.5                                 GLI
4                                  MINIMUM NI
E    0.          1 1
E    .5          1
E    1.          11
END
```

1MATERIALS PROCESSING IN SPACE

MACROSEGREGATION IN A CASTING INGOT

MODEL 2
* UNIDIRECTIONAL SOLIDIFICATION OF A BINARY ALLOY
* UNSTEADY SOLUTION
* PLANAR ISOTHERMS, RECTANGULAR MUSHY ZONE
* ISOTHERM MOVEMENT INPUT
* TEMPERATURE GRADIENT ASSUMED
* NO CONVECTION IN BULK LIQUID
* ISOTROPIC PERMEABILITY K= GAMMA*GL**2

AL 4.5000 CU SOLIDIFICATION MODEL 2 09:55:30 THU, JAN 29 1981

BATCH EXAMPLE
1

ALLOY DATA BASE - DATA BASE REVISED 4/30/80

SOURCE OF INFORMATION FOR AL -CU 0.000E-01 TO 3.300E 01 WT. PCT. CU
PHASE DIAGRAM - M.C. FLEMINGS AND G. NEREO, MET TRANS, VOL 239, 1967, P 1449.
DENSITIES - R. MEHRABIAN, M. KEANE AND M.C. FLEMINGS, TRANS TMS-AIME, VOL 1, 1970, P 1209.
VISCOSITY - R. MEHRABIAN, M. KEANE AND M.C. FLEMINGS, TRANS TMS-AIME, VOL 1, 1970, P 1209.

PHASE DIAGRAM

TEMPERATURE-COMPOSITION SLOPE	-2.860E-01 PCT SOLUTE / DEG C
EQUILIBRIUM PARTITION RATIO	1.720E-01
EUTECTIC COMPOSITION	3.300E 01 PCT SOLUTE
EUTECTIC TEMPERATURE	5.480E 02 DEG C

DENSITIES

COMPOSITION-DENSITY SLOPE	2.670E-02 (GM/CM**3) / PCT SOLUTE
SOLID DENSITY	2.620E 00 GM/CM**3
LIQUID EUTECTIC DENSITY	3.220E 00 GM/CM**3
SOLID EUTECTIC DENSITY	3.400E 00 GM/CM**3

VISCOSITY 3.000E-02 GM/(CM*SEC)

```
AL    4.5000    CU      SOLIDIFICATION MODEL  2     09:55:30    THU, JAN 29 1981

BATCH EXAMPLE

CASE INPUT


SOLIDIFICATION PROCESS PARAMETERS
 1      MOLD (HALF) WIDTH                         2.700E 00      (CM)
 2      MOLD HEIGHT                               6.350E 00      (CM)
 3      ISOTHERM TIME EXPONENT (Q)                1.000E 00
 4      LIQUIDUS ISOTHERM COEFFICIENT (BL)        1.700E-02      (CM/SEC)
 5      EUTECTIC ISOTHERM COEFFICIENT (BE)        1.700E-02      (CM/SEC)
 6      INITIAL ISOTHERM SEPARATION (AE)         -2.000E 00      (CM)
 7      GRAVITATIONAL FORCE                       0.000E-01      (G)

PERMEABILITY MODEL PARAMETERS
 1      GAMMA                                     6.000E-07      (CM**2)

NUMERICAL METHODS CONTROL PARAMETERS
 1      NUMBER OF HORIZONTAL MESH POINTS                 20
 2      NUMBER OF VERTICAL MESH POINTS                    3
 3      MAXIMUM NUMBER OF PRESSURE ITERATIONS           200
 4      PRESSURE CONVERGENCE CRITERION            1.000E-04
 5      FRACTION OF CFL STEP TO TAKE              5.000E-01
 6      MAXIMUM STEP SIZE IN XE                   1.000E-01      (CM)
 7      INITIAL VOLUME FRACTION LIQUID AT CHILL   5.000E-01
 8      MINIMUM HORIZONTAL MESH SIZE                      4


       TIME          STEP SIZE     PRESSURE CYCLES       XE              XL
      15.2939        0.000000            11           -1.74000        0.259996


NEXT CHECKPOINT WILL BE AT T =  117.647     SEC.,  XL =  1.99999    CM.,  XE =-0.108741E-04 CM.


       TIME          STEP SIZE     PRESSURE CYCLES       XE              XL
      21.1762        5.88230             10           -1.64000        0.359995
      27.0585        5.88226             11           -1.54001        0.459994
      32.9408        5.88227             10           -1.44001        0.559992
      38.8230        5.88226              9           -1.34001        0.659991
      44.7052        5.88221             11           -1.24001        0.759988
      50.5875        5.88223             10           -1.14001        0.859986
      56.4697        5.88224              9           -1.04002        0.959983
      62.3518        5.88213             14           -0.940020       1.05998
      68.2340        5.88219             14           -0.840024       1.15998
      74.1161        5.88205             13           -0.740030       1.25997
      79.9981        5.88200             18           -0.640036       1.35996
      85.8801        5.88205             17           -0.540041       1.45996
      91.7621        5.88199             16           -0.440047       1.55995
      97.6441        5.88196             21           -0.340055       1.65994
     103.526         5.88187             20           -0.240063       1.75994
     109.408         5.88193             19           -0.140070       1.85993
     115.290         5.88191             22           -0.400780E-01   1.95992
     117.647         2.35696             26           -0.108741E-04   1.99999
```

AL 4.5000 CU SOLIDIFICATION MODEL 2 09:55:30 THU, JAN 29 1981
BATCH EXAMPLE

TIME = 117.647 SEC

FINAL LOCAL AVERAGE COMPOSITION (WT PCT)

Y/L	
1.00	5.401E 00
0.50	5.401E 00
0.00	5.401E 00

AL 4.5000 CU SOLIDIFICATION MODEL 2 09:55:30 THU, JAN 29 1981
BATCH EXAMPLE

TIME = 117.647 SEC

VOLUME FRACTION LIQUID

(X-XE)/(XL-XE)

Y/L	0.00	0.11	0.22	0.33	0.44	0.56	0.67	0.78	0.89	1.00
1.00	9.171E-02	1.072E-01	1.244E-01	1.433E-01	1.706E-01	2.113E-01	2.730E-01	3.736E-01	5.649E-01	1.000E 00
0.50	9.171E-02	1.072E-01	1.244E-01	1.433E-01	1.706E-01	2.113E-01	2.730E-01	3.736E-01	5.649E-01	1.000E 00
0.00	9.171E-02	1.072E-01	1.244E-01	1.433E-01	1.706E-01	2.113E-01	2.730E-01	3.736E-01	5.649E-01	1.000E 00

NEXT CHECKPOINT WILL BE AT T = 147.059 SEC., XL = 2.49999 CM., XE = 0.499991 CM.

TIME	STEP SIZE	PRESSURE CYCLES	XE	XL
123.528	5.88173	36	0.999780E-01	2.39998
126.624	3.09598	30	0.152611	2.15261
129.720	3.09598	30	0.205244	2.20524
132.816	3.09598	29	0.257873	2.25787
135.912	3.09598	28	0.310504	2.31050
139.008	3.09598	28	0.363134	2.36313
142.104	3.09598	27	0.415768	2.41577
145.200	3.09598	26	0.468397	2.46840
147.059	1.85849	22	0.499991	2.49999

```
------------------------------------------------------------------------------------------------------------
AL     4.5000     CU      SOLIDIFICATION MODEL  2     09:55:30    THU, JAN 29 1981
BATCH EXAMPLE
                                                                                    TIME =  147.059     SEC
FINAL LOCAL AVERAGE COMPOSITION (WT PCT)

 Y/L  *
  *   *    *
 1.00 *  5.326E 00
 0.50 *  5.326E 00
 0.00 *  5.326E 00

NEXT CHECKPOINT WILL BE AT T =  176.470     SEC.,  XL =  2.99999    CM.,  XE = 0.999992    CM.


      TIME          STEP SIZE    PRESSURE CYCLES       XE             XL
     150.155         3.09598           25           0.552622        2.55262
     153.251         3.09598           23           0.605253        2.60525
     156.346         3.09598           23           0.657884        2.65788
     158.823         2.47678           32           0.699989        2.69999
     162.091         3.26799           37           0.755546        2.75555
     165.466         3.37493           37           0.812917        2.81292
     168.730         3.26382           34           0.868404        2.86840
     171.887         3.15713           28           0.922075        2.92207
     175.134         3.24668           23           0.977267        2.97727
     176.470         1.33670           15           0.999992        2.99999

------------------------------------------------------------------------------------------------------------
AL     4.5000     CU      SOLIDIFICATION MODEL  2     09:55:30    THU, JAN 29 1981
BATCH EXAMPLE
                                                                                    TIME =  176.470     SEC
FINAL LOCAL AVERAGE COMPOSITION (WT PCT)

 Y/L  *
  *   *    *
 1.00 *  5.046E 00
 0.50 *  5.046E 00
 0.00 *  5.046E 00

------------------------------------------------------------------------------------------------------------
AL     4.5000     CU      SOLIDIFICATION MODEL  2     09:55:30    THU, JAN 29 1981
BATCH EXAMPLE
                                                                                    TIME =  176.470     SEC
FRACTION EUTECTIC

 Y/L  *
  *   *    *
 1.00 *  8.268E-02
 0.50 *  8.268E-02
 0.00 *  8.268E-02

***** NORMAL TERMINATION
```

SECTION 5
REFERENCES

1. A. L. Maples and D. R. Poirier: "MPS Solidification Model", Volumes I, II and III, General Electric Report No. 80HV007, July, 1980.