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ANALYSIS
OF MAG
CASTING
AND CALCULATION

prepared for MSFC
report no. 88-3875
under contract
no. NAS 8-3375
march 1981

NASA-CR-161720 AS SOLIDIFICATION MODEL
VOLUME 2: OPERATING GUIDE AND SOFTWARE
DOCUMENTATION FOR THE UNSTEADY MODEL
(Geeral Electric Co.) 301 603 AUG 1981
CSER 111

on 2-109

63/20 42117

GENERAL
ELECTRIC

Huntsville, Alabama

the General Electric Co.

space systems division

Huntsville operations

volume 2 - operating guide and software
documentation for the unsteady model
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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
M TO PROCEED TO NEXT CASE.
```

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.
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 bottom 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.

<table>
<thead>
<tr>
<th>Parameter Description</th>
<th>Symbol</th>
<th>Default</th>
<th>Limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mold half width</td>
<td>Xc</td>
<td>2.7 cm</td>
<td>x_c&gt;0</td>
</tr>
<tr>
<td>Mold height</td>
<td>L</td>
<td>6.35 cm</td>
<td>L&gt;0</td>
</tr>
<tr>
<td>Isotherm time exponent</td>
<td>q</td>
<td>1</td>
<td>q&gt;0</td>
</tr>
<tr>
<td>Liquidus coefficient</td>
<td>b_L</td>
<td>0.017 cm/sec</td>
<td>b_L&gt;0</td>
</tr>
<tr>
<td>Eutectic coefficient</td>
<td>b_E</td>
<td>0.017 cm/sec</td>
<td>b_E&gt;0</td>
</tr>
<tr>
<td>Initial separation</td>
<td>a_E</td>
<td>-2 cm</td>
<td>a_E&lt;0</td>
</tr>
<tr>
<td>Gravitational force in -y direction</td>
<td>g</td>
<td>1G</td>
<td>g&gt;0</td>
</tr>
</tbody>
</table>

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 I of this report and Volume I of reference 1.
<table>
<thead>
<tr>
<th>Parameter Description</th>
<th>Symbol</th>
<th>Default</th>
<th>Limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of horizontal mesh points</td>
<td>( N_1 )</td>
<td>20</td>
<td>( 4 &lt; N_1 &lt; 50 )</td>
</tr>
<tr>
<td>Number of vertical mesh points</td>
<td>( N_J )</td>
<td>10</td>
<td>( 3 &lt; N_J &lt; 50 )</td>
</tr>
<tr>
<td>Maximum number of pressure iterations</td>
<td>( M_{SOR} )</td>
<td>200</td>
<td>( M_{SOR} &gt; 0 )</td>
</tr>
<tr>
<td>Pressure convergence criterion</td>
<td>( E_{SOR} )</td>
<td>( 10^{-4} )</td>
<td>( E_{SOR} &gt; 5 \times 10^{-6} )</td>
</tr>
<tr>
<td>Fraction of CFL step to take</td>
<td>( f )</td>
<td>.5</td>
<td>( 0 &lt; f &lt; 1 )</td>
</tr>
<tr>
<td>Maximum step size in ( x_E )</td>
<td>( \Delta x_E )</td>
<td>.1 cm</td>
<td>( \Delta x_E &gt; 0 )</td>
</tr>
<tr>
<td>Initial ( g_L ) at chill</td>
<td>( g_{L1} )</td>
<td>.9</td>
<td>( .1 &lt; g_{L1} &lt; 1 )</td>
</tr>
<tr>
<td>Minimum horizontal mesh size</td>
<td>( N_{\text{imin}} )</td>
<td>4</td>
<td>( 4 &lt; N_{\text{imin}} &lt; 50 )</td>
</tr>
</tbody>
</table>
3.1 FLOW DIAGRAMS

3.1.1 Global Flow Diagram

BEGIN

INPUT 1 CASE

INITIALIZE CALCULATION

ADVANCE SOLUTION 1 STEP IN TIME

CHECKPOINT OR FINISHED

INTERACTIVE OUTPUT
- TABLES
- GRAPHS
BATCH OUTPUT
- TABLES

FINISHED OR USER SELECTED NEXT CASE

USER SELECTED QUIT

INPUT NEXT CHECKPOINT

STOP
3.1.2 Calculation

BEGIN

- INITIALIZE PROGRAM CONSTANTS (INIT)

INPUT SECTION

- INITIALIZE CURRENT CASE (INIT)

TAKE 1 STEP AWAY FROM CHILL (START)

- DETERMINE TIME STEP SIZE, Δt (STEP)

- ADVANCE S_L AND 1 STEP (STEP)

\[ t_{n+1} = t_n + \Delta t \]

- SET UP MESH, T, \( \rho_L \), \( C_L \) AT \( t \) (EVAL)
- EVALUATE \( K \), \( C_S(x_E) \)

- CALCULATE PRESSURE FIELD AT \( t \) (PSETUP, PSOLVE)

- CALCULATE VELOCITY AT \( t \) AND CHECK FOR FRECKLING (VLCTY)

OUTPUT SECTION

FINISHED

- NO OR USER SELECTED NEXT CASE

YES
3.1.3 Input Section

CONTROLLER: INCON
CALLED FROM: INIT

INITIALIZE INPUT ARRAYS (INCON)

INITIALIZE TERMINAL CONTROL SYSTEM (IACTI)

PUT ID PAGE ON SCREEN AND GET CASE TITLE (IACTI)

GET ALLOY (IACTI)

ACCESS ALLOY DATA BASE (ADB)

GET REMAINING PARAMETERS (IACTI)

READ CASE TITLE (BATCHI)

END OF FILE?

YES STOP

READ AND PRINT ALLOY (BATCHI)

ACCESS ALLOY DATA BASE (ADB)

READ AND PRINT REMAINING PARAMETERS (BATCHI)

INPUT ERRORS IN THIS CASE?

YES

EXTRACT PARAMETER VALUES FROM INPUT ARRAYS (INCON)

CONVERT TO CGS UNITS (INCON)

RETURN
3.1.4 Output Section

CONTROLLER: TMCON
CALLED FROM: Main

YES PRINT TABLESBATCH?	 (ADISP)
NO
RETURN

GET USER SELECTED ACTION

G
Q
STOP
P
RETURN

GET USER SELECTED ACTION
(GPHCON)

ITEM # OF FUNCTION TO PLOT

GET USER SELECTED ACTION
(GPHCON)

ITEM # OF PLOT TYPE

CALCULATE NEAT SCALING (SCALE)

INITIALIZE PLOT, PUT ON LABELS (SETPLT)

PUT ON PARAMETER BLOCK (GPHBLK)

DRAW AXES (AXES)

PLOT CONTROLLS BY CTR, HPROFS, VPROFS, OR VECPLT

DISPLAY TABLES ON SCREEN (ADISP)

3-4
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.

<table>
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<tr>
<th>NAME</th>
<th>SECTION</th>
<th>FUNCTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADB</td>
<td>I/O</td>
<td>Retrieve phase diagram, densities and viscosity from alloy data base.</td>
</tr>
<tr>
<td>ADISP</td>
<td>I/O</td>
<td>Displays any array on the screen or in printed form.</td>
</tr>
<tr>
<td>ALNUIN</td>
<td>I/O</td>
<td>Gets interactive input that may be either alphanumeric or numerical.</td>
</tr>
<tr>
<td>AXES</td>
<td>Graphics</td>
<td>Draws and labels axes on all plots.</td>
</tr>
<tr>
<td>BATCHI</td>
<td>I/O</td>
<td>Controls batch mode card input.</td>
</tr>
<tr>
<td>COORD</td>
<td>Calculation</td>
<td>Calculates isotherm positions and coordinate transformation.</td>
</tr>
<tr>
<td>CTR</td>
<td>Graphics</td>
<td>Controls contour plots.</td>
</tr>
<tr>
<td>CTRBOX</td>
<td>Graphics</td>
<td>Logic for contouring over given rectangular region.</td>
</tr>
<tr>
<td>CTRDRW</td>
<td>Graphics</td>
<td>Draws contour line elements.</td>
</tr>
<tr>
<td>CTRLAB</td>
<td>Graphics</td>
<td>Labels contour level values.</td>
</tr>
<tr>
<td>DISKC</td>
<td>I/O</td>
<td>Performs various control functions on disk files.</td>
</tr>
<tr>
<td>DISKI</td>
<td>I/O</td>
<td>Retrieves final solid data from temporary disk for use by graphics routines.</td>
</tr>
<tr>
<td>DISKO</td>
<td>I/O</td>
<td>Writes final solid data on temporary disk.</td>
</tr>
<tr>
<td>EVAL</td>
<td>Calculation</td>
<td>Evaluates specified functions at current time.</td>
</tr>
<tr>
<td>GPBLK</td>
<td>Graphics</td>
<td>Puts parameter block on plot.</td>
</tr>
<tr>
<td>GPHCON</td>
<td>Graphics</td>
<td>Controls interactive graphics.</td>
</tr>
<tr>
<td>GRIDCN</td>
<td>Calculation</td>
<td>Controls size of computational grid.</td>
</tr>
<tr>
<td>GRIDXE</td>
<td>Calculation</td>
<td>Sets up computational grid.</td>
</tr>
<tr>
<td>HPROFS</td>
<td>Graphics</td>
<td>Controls horizontal profile plots.</td>
</tr>
<tr>
<td>IACTI</td>
<td>I/O</td>
<td>Controls interactive input.</td>
</tr>
<tr>
<td>INCON</td>
<td>I/O</td>
<td>Controls input section.</td>
</tr>
<tr>
<td>INIT</td>
<td>Calculation</td>
<td>Initialization routine.</td>
</tr>
<tr>
<td>MASSCK</td>
<td>I/O</td>
<td>Monitors conservation of mass.</td>
</tr>
<tr>
<td>MSG</td>
<td>I/O</td>
<td>Puts any brief message on terminal screen.</td>
</tr>
<tr>
<td>NAME</td>
<td>SECTION</td>
<td>FUNCTION</td>
</tr>
<tr>
<td>-------</td>
<td>------------------</td>
<td>----------------------------------------------------</td>
</tr>
<tr>
<td>PERM</td>
<td>Calculation</td>
<td>Calculates permeability.</td>
</tr>
<tr>
<td>PSETUP</td>
<td>Calculation</td>
<td>Calculates A, and B and sets up boundary conditions (see equations 1.3.4.4 to 1.3.4.11)</td>
</tr>
<tr>
<td>PSOLVE</td>
<td>Calculation</td>
<td>Solves the pressure equation (see reference 1, Vol. 1, 4.5)</td>
</tr>
<tr>
<td>SCALE</td>
<td>1/0</td>
<td>Calculates neat scales for plots.</td>
</tr>
<tr>
<td>SETHOL</td>
<td>1/0</td>
<td>Sets up long hollerith arrays.</td>
</tr>
<tr>
<td>SETPLT</td>
<td>Output</td>
<td>Initializes all plots and puts on labels.</td>
</tr>
<tr>
<td>START</td>
<td>Calculation</td>
<td>Takes first step away from chill. (See Vol. 1, Section 4.3)</td>
</tr>
<tr>
<td>STEP</td>
<td>Calculation</td>
<td>Advances qL and I one step (See Vol 1, Section 4.4)</td>
</tr>
<tr>
<td>TABCON</td>
<td>1/0</td>
<td>Controls tabular output</td>
</tr>
<tr>
<td>TMCON</td>
<td>1/0</td>
<td>Controls display checkpoints and time-varying I/O.</td>
</tr>
<tr>
<td>VECPLT</td>
<td>Output</td>
<td>Controls plots of vector fields.</td>
</tr>
<tr>
<td>VCLCTY</td>
<td>Calculation</td>
<td>Calculates velocity.</td>
</tr>
<tr>
<td>VPROFS</td>
<td>Output</td>
<td>Controls vertical profile plots.</td>
</tr>
<tr>
<td>WAIT</td>
<td>Output</td>
<td>Waits for the operator to enter a P.</td>
</tr>
</tbody>
</table>

### 3.3 KEY PROGRAM SYMBOLS

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

<table>
<thead>
<tr>
<th>PROGRAM SYMBOL</th>
<th>COMMON BLOCK</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>AE</td>
<td>/PROCESS</td>
<td>aE</td>
</tr>
<tr>
<td>AGC</td>
<td>/SLZONE</td>
<td>I</td>
</tr>
<tr>
<td>ALNAM</td>
<td>/ALLOY</td>
<td>Element 1 is the hollerith solvent name. Element 2 is the hollerith solute name.</td>
</tr>
<tr>
<td>BE, BL</td>
<td>/PROCESS</td>
<td>bE, bL</td>
</tr>
<tr>
<td>CL</td>
<td>/SLZONE</td>
<td>C_L</td>
</tr>
<tr>
<td>CL0</td>
<td>/ALLOY</td>
<td>C_0</td>
</tr>
<tr>
<td>DCLDT</td>
<td>/ALLOY</td>
<td>dC_L/dT</td>
</tr>
<tr>
<td>DRHDC</td>
<td>/ALLOY</td>
<td>dP_L/dC_L</td>
</tr>
<tr>
<td>DTM</td>
<td>/SLZONE</td>
<td>∆T/∆t = ε</td>
</tr>
<tr>
<td>DXI</td>
<td>/MESH</td>
<td>∆ξ</td>
</tr>
<tr>
<td>DET</td>
<td>/MESH</td>
<td>∆η</td>
</tr>
<tr>
<td>EPR</td>
<td>/ALLOY</td>
<td>k</td>
</tr>
</tbody>
</table>

3-6
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 TC5500
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
OPEN ICARD 1 1
CO -END

Command File MPS2.BATCH
OPEN CARDS 1 1
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 database 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.
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, $C_s = 4.5\%$ 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 preceding 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

MICROSEGREGATION IN A CASTING INGOT

MODEL B
1. UNIDIRECTIONAL SOLIDIFICATION OF A BINARY ALLOY
2. UNSTEADY SOLUTION
3. PLANAR ISOTHERMS, RECTANGULAR MUSHY ZONE
4. ISOTHERMAL MOVEMENT INPUT
5. TEMPERATURE GRADIENT ASSUMED
6. NO CONVECTION IN BULK LIQUID
7. ISOTROPIC PERMEABILITY k = GAMMAGLBB

ENTER CASE TITLE (UP TO 80 CHARACTERS)

.................................

ALLOY

SOLUTE: 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:
- 8.000E-01 TO 3.300E 01 UT. PCT. Cu

PHASE DIAGRAM
- TEMPERATURE-COMPOSITION SLOPE
- EQUILIBRIUM PARTITION RATIO
- EUTECTIC COMPOSITION
- EUTECTIC TEMPERATURE

DENSITIES
- COMPOSITION-DENSITY SLOPE
- SOLID DENSITY
- LIQUID EUTECTIC DENSITY
- SOLID EUTECTIC DENSITY

VISCOSITY

ENTER P TO PROCEED

P

4-2
### SOLIDIFICATION過程參數

<table>
<thead>
<tr>
<th>參數</th>
<th>價值</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. 納鐵模寬度</td>
<td>8.708E-08 (CM)</td>
</tr>
<tr>
<td>2. 模高</td>
<td>6.356E-08 (CM)</td>
</tr>
<tr>
<td>3. 等溫面時間指數 (Q)</td>
<td>1.988E-08</td>
</tr>
<tr>
<td>4. 液相等溫面係數 (IL)</td>
<td>1.280E-02 (CM/SEC)</td>
</tr>
<tr>
<td>5. 等溫面係數 (BE)</td>
<td>1.280E-02 (CM/SEC)</td>
</tr>
<tr>
<td>6. 初期等溫面分離 (AE)</td>
<td>-8.000E-08 (CM)</td>
</tr>
<tr>
<td>7. 重力作用力</td>
<td>1.000E-08 (G)</td>
</tr>
</tbody>
</table>

### PERMEABILITY模型參數

<table>
<thead>
<tr>
<th>參數</th>
<th>價值</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. GAMMA</td>
<td>6.000E-07 (CM**8/8)</td>
</tr>
</tbody>
</table>

### NUMERICAL METHODS控制參數

<table>
<thead>
<tr>
<th>參數</th>
<th>價值</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. 水平網格點數</td>
<td>80</td>
</tr>
<tr>
<td>2. 垂直網格點數</td>
<td>10</td>
</tr>
<tr>
<td>3. 最大壓力迭代次數</td>
<td>880</td>
</tr>
<tr>
<td>4. 壓力收玫標準</td>
<td>1.000E-04</td>
</tr>
<tr>
<td>5. CF1步長比例</td>
<td>5.000E-01</td>
</tr>
<tr>
<td>6. 最大步長 X</td>
<td>1.000E-01</td>
</tr>
<tr>
<td>7. 初期液體體積比例</td>
<td>9.000E-01 (CM)</td>
</tr>
<tr>
<td>8. 最小水平網格尺寸</td>
<td>4</td>
</tr>
</tbody>
</table>

Enter item number to change, or P to proceed.
### Calculation in Progress for Case

**AL  4.5000   CU**

**SOLIDIFICATION MODEL 2   09:00:00   THU, JAN 81, 1981**

<table>
<thead>
<tr>
<th>TIME</th>
<th>STEP SIZE</th>
<th>PRESSURE CYCLES</th>
<th>XE</th>
<th>XL</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.88834</td>
<td>0.04175</td>
<td>11</td>
<td>-1.968</td>
<td>0.39993E-01</td>
</tr>
</tbody>
</table>

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 = 1.88834 SEC.**

Liquidus isotherm is 0.39993E-01 cm from chill.

Eutectic isotherm is -1.9680 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.

<table>
<thead>
<tr>
<th>TIME</th>
<th>STEP SIZE</th>
<th>PRESSURE CYCLES</th>
<th>XE</th>
<th>XL</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.82351</td>
<td>0.94175</td>
<td>10</td>
<td>-1.968</td>
<td>0.47993E-01</td>
</tr>
<tr>
<td>4.22577</td>
<td>1.14175</td>
<td>17</td>
<td>-1.968</td>
<td>0.71999E-01</td>
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<tr>
<td>6.61760</td>
<td>1.32552</td>
<td>14</td>
<td>-1.968</td>
<td>0.11999E-01</td>
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<tr>
<td>8.27200</td>
<td>1.65445</td>
<td>23</td>
<td>-1.968</td>
<td>0.14999E-01</td>
</tr>
<tr>
<td>9.65866</td>
<td>1.79567</td>
<td>22</td>
<td>-1.968</td>
<td>0.15999E-01</td>
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<tr>
<td>11.2951</td>
<td>1.86844</td>
<td>21</td>
<td>-1.968</td>
<td>0.19999E-01</td>
</tr>
<tr>
<td>14.386</td>
<td>1.87653</td>
<td>26</td>
<td>-1.7766</td>
<td>0.22330E-01</td>
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<tr>
<td>14.7776</td>
<td>1.64106</td>
<td>26</td>
<td>-1.7488</td>
<td>0.26121E-01</td>
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<tr>
<td>245.521</td>
<td>8.31308</td>
<td>28</td>
<td>8.1730</td>
<td>4.7328</td>
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<tr>
<td>247.391</td>
<td>1.85958</td>
<td>28</td>
<td>8.2864</td>
<td>4.8964</td>
</tr>
<tr>
<td>249.101</td>
<td>1.71989</td>
<td>87</td>
<td>8.8347</td>
<td>4.8347</td>
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<tr>
<td>250.958</td>
<td>1.85784</td>
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<td>8.8668</td>
<td>4.8668</td>
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<tr>
<td>252.653</td>
<td>1.69482</td>
<td>88</td>
<td>8.8910</td>
<td>4.8910</td>
</tr>
<tr>
<td>254.139</td>
<td>1.54536</td>
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<td>8.3813</td>
<td>4.3813</td>
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<tr>
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<td>4.3799</td>
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<td>258.765</td>
<td>1.35549</td>
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<td>4.3900</td>
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<tr>
<td>260.264</td>
<td>1.51278</td>
<td>82</td>
<td>8.4248</td>
<td>4.4248</td>
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<tr>
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<td>4.4478</td>
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<td>4.4666</td>
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<td>264.874</td>
<td>1.32634</td>
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<td>8.4916</td>
<td>4.4916</td>
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<tr>
<td>265.168</td>
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<td>4.5879</td>
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<td>8.6894</td>
<td>4.6894</td>
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<tr>
<td>267.169</td>
<td>1.11388</td>
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<td>8.5418</td>
<td>4.5418</td>
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<tr>
<td>267.982</td>
<td>0.812863</td>
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<td>4.5659</td>
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<tr>
<td>268.576</td>
<td>0.593910</td>
<td>10</td>
<td>8.5687</td>
<td>4.5687</td>
</tr>
<tr>
<td>269.008</td>
<td>0.432339</td>
<td>10</td>
<td>8.5783</td>
<td>4.5783</td>
</tr>
</tbody>
</table>

SOLIDIFICATION COMPLETE.

Enter T to display tabular data,
G to display graphs,
Q to terminate run, or
N to proceed to next case.

G
FUNCTION TO PLOT

S/L ZONE

1 VELOCITY
2 PRESSURE - BULK HYDROSTATIC P
3 FRACTION LIQUID
4 MASS FLOW
5 SOLUTE 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.

ENTER ITEM NUMBER OF PLOT TYPE

FUNCTION MINIMUM = 0.774 FUNCTION MAXIMUM = 6.30
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.

ENTER BASE LEVEL

4.5

ENTER LEVEL INTERVAL

.25

FUNCTION MINIMUM = 0.774 FUNCTION MAXIMUM = 6.30
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
P TO CHANGE LEVELS
Al 4.5000 Cu 4.5000
SOLIDIFICATION MODEL 8

FUNCTION TO PLOT

S/L ZONE
1 VELOCITY
2 PRESSURE - P-Po
3 FRACTION LIQUID
4 MASS FLOW
5 SOLUTE FLOW

7 FINAL LOCAL AVERAGE COMPOSITION
8 VOLUME FRACTION EUTECTIC

PLOT TYPE
1 VERTICAL PROFILES
2 HORIZONTAL PROFILES
3 VECTOR FIELD
4 CONTOURS

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

ENTER ITEM NUMBER OF PLOT TYPE

MINIMUM FUNCTION VALUE IS 0.774600
MAXIMUM FUNCTION VALUE IS 5.29138

AUTOMATIC SCALING YIELDS PLOT RANGE: 2.500 TO 6.500 WITH REMOTE EXPONENT 0
OVER 5 MAJOR TIC INTERVALS

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

ENTER Y VALUE OF PROFILE OR
P TO PROCEED.

ENTER Y VALUE OF PROFILE OR
P TO PROCEED.

ENTER Y VALUE OF PROFILE OR
P TO PROCEED.

ENTER Y VALUE OF PROFILE OR
P TO PROCEED.
FUNCTION TO PLOT

SOLIDIFICATION MODEL 2

PLOT TYPE

VELOCITY
PRESSURE - BULK HYDROSTATIC P
FRACTION LIQUID
MASS FLOW
SOLUTE FLOW

INGOT

FINAL LOCAL AVERAGE COMPOSITION
VOLUME FRACTION (UTECTIC)

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

ENTER ITEM NUMBER OF PLOT TYPE

MINIMUM FUNCTION VALUE IS 0.774888E-03
MAXIMUM FUNCTION VALUE IS 5.29538E-03

AUTOMATIC SCALING YIELDS PLOT RANGE: 2.500 TO 6.500 WITH REMOTE EXPONENT 0
OVER 5 MAJOR TIC INTERVALS

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

ENTER REMOTE EXPONENT

ENTER NUMBER OF MAJOR TIC INTERVALS.

FINAL SOLID FORMED BETWEEN X = -0.106741E-04 AND X = 2.780000 CM. FROM CHILL.

ENTER X VALUE OF PROFILE OR P TO PROCEED.

ENTER X VALUE OF PROFILE OR P TO PROCEED.

ENTER X VALUE OF PROFILE OR P TO PROCEED.
Enter 7 to display tabular data.
6 to display graphs,
8 to terminate run, or
m to proceed to next case.

AL 4.5000 CU SOLIDIFICATION MODEL 8 09:08:08 THU, JAN 08 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  B  06/22/69  UCD, DEC 04 1989

PASS BALANCE AT TIME =  859.000  DEC.
KE =  4.57311  CR.
KE =  2.57311  CR.

<table>
<thead>
<tr>
<th>METAL PASS (GN)</th>
<th>SOLUTE PASS (GN)</th>
<th>AVERAGE PERCENT SOLUTE</th>
</tr>
</thead>
<tbody>
<tr>
<td>CURRENT FINAL SOLID</td>
<td>45.2336</td>
<td>2.10974</td>
</tr>
<tr>
<td>CUMULATIVE FLOW THROUGH LIQUIDUS ISOHERN</td>
<td>46.7374</td>
<td>2.95556</td>
</tr>
<tr>
<td>- CURRENT S/L ZONE CONTENTS</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| CURRENT S/L ZONE CONTENTS | 0.000000 | 0.000000 | 0.000000 |
| PREVIOUS S/L ZONE CONTENTS | -0.181735E-02 | -8.457805E-03 | 0.000000 |
| + FLOW IN THROUGH LIQUIDUS ISOHERN | | | |
| - FLOW OUT THROUGH EUTECTIC ISOHERN | | | |

| CURRENT BULK MOLT CONTENTS | 0.004380 | 0.000000 | 0.000000 |
| INITIAL MOLT CONTENTS | -3.57898 | -8.109994 | 4.59294 |
| - CUMULATIVE FLOW THROUGH LIQUIDUS | | | |

| CURRENT MOLT CONTENTS | 45.2336 | 2.10974 | 4.5333 |
| INITIAL MOLT CONTENTS | 46.1884 | 1.89788 | 4.58888 |

ORIGINAL PAGE IS OF POOR QUALITY

4-12
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
4.5
2.7
6.35
1.
.017
.017
2.
0
6.E-7
20
3
200
1.E-4
.5
1
4
E  0.  11
E .5  1
E 1.  11
END

MOLD HALF WIDTH (CM)
MOLD HEIGHT (CM)
BL
BE
GRAVITY (G)
NUMBER OF HORIZONTAL MESH POINTS
NUMBER OF VERTICAL MESH POINTS
MAXIMUM NUMBER OF PRESSURE ITERATIONS
PRESSURE CONVERGENCE BOUND
FRACTION OF CFL STEP
MAXIMUM STEP IN XE
GLI
MINIMUM NI
```
INMATERIALS PROCESSING IN SPACE

MACROSEGREGATION IN A CASTING INGOT

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

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
TEMPERATURE-COMPOSITION SLOPE -2.88E-01 PCT SOLUTE / DEG C
EQUILIBRIUM PARTITION RATIO 1.72E-01
EUTECTIC COMPOSITION 3.30E 01 PCT SOLUTE
EUTECTIC TEMPERATURE 5.48E 02 DEG C

DENSITIES
COMPOSITION-DENSITY SLOPE 2.670E-02 (GM/CM3) / PCT SOLUTE
SOLID DENSITY 2.620E 00 GM/CM3
LIQUID EUTECTIC DENSITY 3.220E 00 GM/CM3
SOLID EUTECTIC DENSITY 3.40E 00 GM/CM3

VISCOSITY 3.00E-02 GM/(CMSSEC)
**SOLIDIFICATION PROCESS PARAMETERS**

1. MOLD (HALF) WIDTH: 8.700E 00 (CM)
2. MOLD HEIGHT: 6.350E 00 (CM)
3. ISOTHERM TIME EXPONENT (G): 1.600E 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/SEC)

**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

<table>
<thead>
<tr>
<th>TIME</th>
<th>STEP SIZE</th>
<th>PRESSURE CYCLES</th>
<th>XE</th>
<th>XL</th>
</tr>
</thead>
<tbody>
<tr>
<td>15.2939</td>
<td>0.000000</td>
<td>11</td>
<td>-1.74000</td>
<td>0.250006</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>TIME</th>
<th>STEP SIZE</th>
<th>PRESSURE CYCLES</th>
<th>XE</th>
<th>XL</th>
</tr>
</thead>
<tbody>
<tr>
<td>21.1762</td>
<td>5.88230</td>
<td>10</td>
<td>-1.64000</td>
<td>0.359925</td>
</tr>
<tr>
<td>27.9555</td>
<td>5.88226</td>
<td>11</td>
<td>-1.54001</td>
<td>0.45999</td>
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<tr>
<td>32.9480</td>
<td>5.88227</td>
<td>10</td>
<td>-1.44001</td>
<td>0.559992</td>
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<tr>
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<td>9</td>
<td>-1.34001</td>
<td>0.65999</td>
</tr>
<tr>
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<td>-1.24001</td>
<td>0.759988</td>
</tr>
<tr>
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<td>-1.14001</td>
<td>0.859986</td>
</tr>
<tr>
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<td>5.88244</td>
<td>9</td>
<td>-1.04002</td>
<td>0.959983</td>
</tr>
<tr>
<td>62.3512</td>
<td>5.88213</td>
<td>14</td>
<td>-0.94020</td>
<td>1.05998</td>
</tr>
<tr>
<td>68.2340</td>
<td>5.88219</td>
<td>14</td>
<td>-0.84024</td>
<td>1.15998</td>
</tr>
<tr>
<td>74.1151</td>
<td>5.88305</td>
<td>13</td>
<td>-0.74038</td>
<td>1.25997</td>
</tr>
<tr>
<td>79.0981</td>
<td>5.88200</td>
<td>18</td>
<td>-0.64086</td>
<td>1.35996</td>
</tr>
<tr>
<td>85.8801</td>
<td>5.88205</td>
<td>17</td>
<td>-0.54084</td>
<td>1.45996</td>
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FINAL LOCAL AVERAGE COMPOSITION (WT PCT)

Y/L 1
1.00 x 5.401E 00
0.50 x 5.401E 00
0.00 x 5.401E 00

VOLUME FRACTION LIQUID

Y/L 1
1.00 x 9.171E-02 1.072E-01 1.244E-01 1.433E-01 1.706E-01 2.113E-01 2.738E-01 3.736E-01 5.649E-01 1.088E 00
0.50 x 9.171E-02 1.072E-01 1.244E-01 1.433E-01 1.706E-01 2.113E-01 2.738E-01 3.736E-01 5.649E-01 1.088E 00
0.00 x 9.171E-02 1.072E-01 1.244E-01 1.433E-01 1.706E-01 2.113E-01 2.738E-01 3.736E-01 5.649E-01 1.088E 00

NEXT CHECKPOINT WILL BE AT T = 147.059 SEC., XL = 2.49999 CM., XE = 0.49999 CM.
FINAL LOCAL AVERAGE COMPOSITION (WT PCT)

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

FRACTION EUTECTIC

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NORMAL TERMINATION
SECTION 5
REFERENCES