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Controlled Thermonuclear Reactor (CTR)

by

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HEAT TRANSFER MODEL FOR COMPOSITE FIRST WALL MATERIALS IN A PULSED HIGH-BETA  
CONTROLLED THERMONUCLEAR REACTOR  
(CTR)

by

Jefferson W. Tester and C. C. Herrick

ABSTRACT

A computer model has been constructed to predict temperature and time excursions for radial composite walls currently under consideration for pulsed high-beta Z-pinch machines. The effects of incident flux, internal heat distribution functions, thermal properties, and material dimensions have been examined for a Nb/Al<sub>2</sub>O<sub>3</sub> composite to establish the feasibility of the model.

I. INTRODUCTION AND SCOPE

In a previous report,<sup>1</sup> a preliminary treatment of first wall heat transfer and chemical stability effects was presented. For homogeneous materials such as Nb, Al<sub>2</sub>O<sub>3</sub>, BeO, or BN temperature excursions and/or chemical reactivity with molecular or atomic hydrogen became prohibitive, indicating that a composite first wall might present a feasible alternative. Prediction of thermodynamic equilibrium, kinetic, thermal stressing, and radiation damage effects require first-hand knowledge of anticipated temperature-time profiles for composite wall materials intended for use in pulsed, high-beta, controlled thermonuclear reactors (CTR's) where heat fluxes on the order of 1 kW/cm<sup>2</sup> or more are possible. Furthermore, estimates of maximum operating temperatures for the molten lithium blanket are useful in establishing the effectiveness of proposed CTR's in producing high temperature heat sources for direct or indirect energy production.

II. DESCRIPTION OF THE MODEL

A. Basic Geometry

Due to the large radius of curvature (30 m) and torus diameter (~ 1 m) a rectangular coordinate system was used for the model. Figure 1 illustrates schematically how a Z-pinch prototype might be

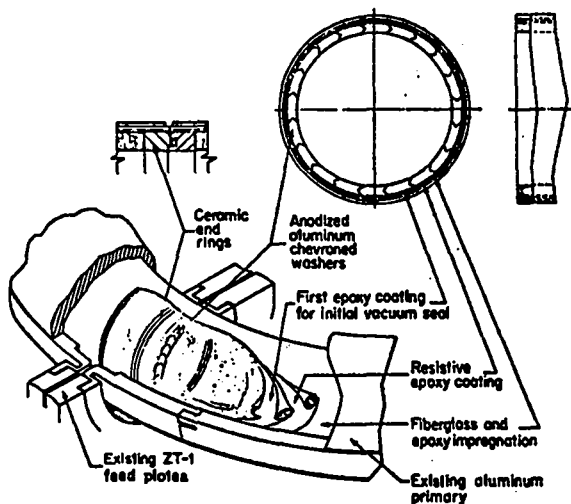


Fig. 1. Schematic of prototype Z-pinch design.<sup>2</sup>

designed.<sup>2</sup> The major feature of interest is the radial arrangement of the composite first wall. In the prototype design the conductor (material 1) is an aluminum washer separated by thin layers of anodized aluminum which can be conceptually thought of as the insulator (material 2). Figures 2A and 2B schematically represent the geometry used in the model. The grid has 12 points in the x-direction and J

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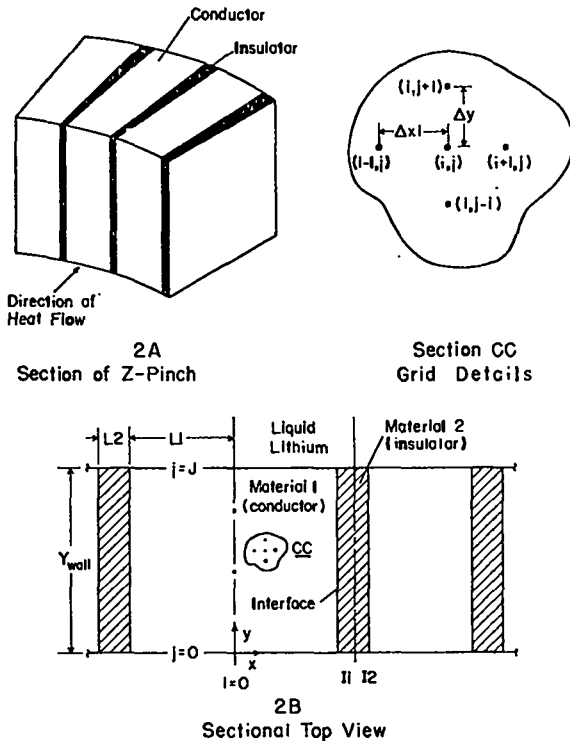


Fig. 2. Geometry employed for finite difference grid.  $I_2 \times J$  points having  $\Delta y$  spacing in the  $y$ -direction and  $\Delta x_1 (\Delta x_2)$  spacing in the  $x$ -direction for materials 1(2).

points in the  $y$ -direction with the point at  $I_1$  on the interface between materials 1 and 2.

A time-dependent heat flux impinges on the inner surface of the composite [ $i=0, \dots, I_1, \dots, I_2; j=0$ ], and a liquid metal (lithium)/metal conduction temperature dependent heat transfer resistance exists on the outer surface [ $i=0, \dots, I_1, \dots, I_2; j=J$ ]. The two center lines (---) define mirror symmetry planes in each material and can be represented by a zero flux [ $-k \frac{\partial T}{\partial x} = 0$ ] condition.

### B. Design Criteria

Heat enters the first wall via several sources, including:

1. Bremsstrahlung radiation,
2.  $n-\gamma$  reactions within the wall, and
3. direct neutron deposition energy.

In a preliminary report, Burnett, Ellis, Oliphant, and Ribe<sup>3</sup> demonstrated that most of the energy deposited ( $> 85\%$ ) was Bremsstrahlung energy. In our model, the total heat absorbed is divided

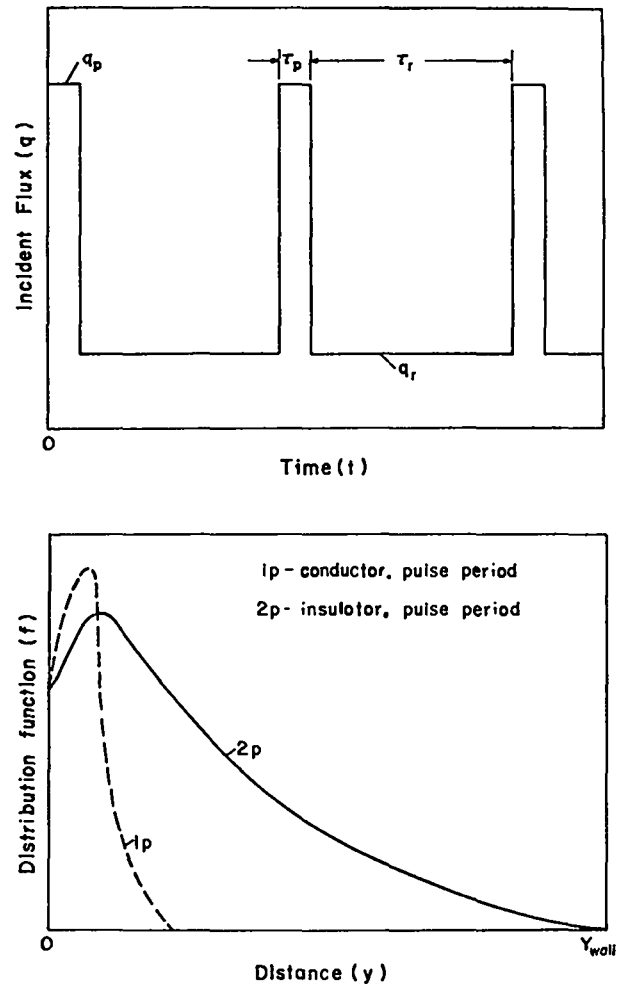


Fig. 3. Incident heat flux  $q$  and heat distribution functions  $f = H(y)/q_p \Delta y$  expressed as a fraction of the pulse heat flux  $q_p$  (arbitrary scales).

into two quantities:

1. An incident flux which is deposited at the surface  $y = 0$ .
2. A distributed heat source function  $H = f(y)$  representing the energy absorbed as a function of distance into the wall from the point  $y = 0$  to the extent of the wall  $y = Y_{wall}$ .

Consequently, for a two-component composite, there would be four  $H$  functions corresponding to each material in the pulse and rest mode. In Fig. 3, we present idealizations of these heat distribution and incident flux functions used in the current approach.

Only distribution  $H(y)$  curves for the pulse period are shown in Fig. 3, since negligible values for the rest period are anticipated when heat transfer to the wall will be primarily by radiation and convection from the expanding plasma. As a first approximation, one might assume that  $H(y)/q = 0$  during the rest period for both materials, indicating that all of the heat is deposited on the inside surface of the wall. Nevertheless, in implementing the model, the user is free to select any heat distribution function that is appropriate. For example, for our Nb/Al<sub>2</sub>O<sub>3</sub> composite both rest and pulse  $H$  functions are set to zero for Nb, and a finite  $H$  used only for the pulse mode in Al<sub>2</sub>O<sub>3</sub> (see Ref. 3). In general, the insulator (ceramic) would be expected to have a much wider distribution function than the conductor (metal) as is illustrated in Fig. 3.

The square wave function idealization for  $q$  is somewhat of an over-simplification of the actual case which might show an exponential increase and decrease of heat flux during the cycle.<sup>4</sup> However, at this stage, a square wave functionality should be adequate. Actual values for the incident heat flux  $q$  may be determined by design limitations of the materials used in the first wall. For example, the magnitude of  $q$  can be partially controlled by changing the amount of first wall surface area for a given amount of heat produced during the cycle.

### C. Governing Equations and Boundary Conditions

The following partial differential equation (PDE) applicable to unsteady state, two-dimensional heat conduction was used for both materials.

$$\alpha_i \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] + \frac{H_i(y)}{\rho_i C_{p_i}} = \frac{\partial T}{\partial t} \quad (1)$$

$i = 1, 2$  (for both materials).

An ambient temperature ( $T_B$ ) equal to the bulk lithium temperature is assumed for the initial condition at  $t = 0$ . Four boundary conditions are applied to positions specified on Fig. 2B:

1. Incident heat flux at the inside surface (see Fig. 3)

at  $y = 0$  ( $j = 0$ ), all  $x$

$$-k_i \left( \frac{\partial T}{\partial y} \right) = q_i(t)^\dagger \quad (2)$$

2. Temperature dependent flux with contact resistance at the outside surface

at  $y = 0$  ( $j = 0$ ), all  $x$

$$-k_i \left( \frac{\partial T}{\partial y} \right) = h (T - T_B)^\dagger \quad (3)$$

where  $h$  is an effective heat transfer coefficient applying to the molten lithium blanket and any solid liners that might be used.

3. Continuous flux and temperature at the interface

at  $x = L1/2$  ( $i = I1$ ), all  $y$

$$k1 \left( \frac{\partial T}{\partial x} \right) = k2 \left( \frac{\partial T}{\partial x} \right) \quad (4)$$

4. Zero flux condition at centerlines of materials 1 and 2 via symmetry

$$\text{at } x = 0: (i = 0), \left( \frac{\partial T}{\partial x} \right) = 0 \quad (5)$$

$$\text{at } x = \frac{(L1 + L2)}{2} (i = I2) \left( \frac{\partial T}{\partial x} \right) = 0 \quad (6)$$

In solving Eq. (1) to generate temperature profiles as functions of time, a dimensionless temperature  $u$  was defined as

$$u \equiv \frac{T - T_B}{T_B} \quad (7)$$

and finite difference equations were written to approximate the PDE. Appendix A contains a tabular presentation of these equations. A detailed description of the finite difference formulation of the boundary conditions is presented in Appendix B. An Alternating Direction Implicit (ADI) scheme was used to solve the system of equations (see Appendix C). The advantages of an implicit rather than explicit scheme should be useful in conserving machine time and in adding to the flexibility of the code.

<sup>†</sup> In the expression  $k_i$  or  $q_i$  the  $i = 1$  or  $2$  depending on what material it is.

The tridiagonal algorithm and a complete listing of the Madcap V code are presented in Appendixes D and E.

### III. LIMITATIONS AND APPLICATIONS OF THE MODEL

Several features of the model have been kept general; for example, various wall sizes can be used with any two materials. If the repeating thicknesses in the  $x$ -direction,  $L1$  and  $L2$ , become much smaller than the thickness of the wall in the  $y$ -direction  $Y_w$ , the code reverts to a unidirectional ( $y$  only) calculation of temperature profiles with area average physical properties used. Any combination of incident heat flux and internal heat generation terms can be used. The outside boundary condition (all  $x$ ,  $y = Y_{wall}$  at  $j = J$ ) is temperature dependent in order that an effective heat transfer coefficient can be used which combines the resistances of a liquid lithium boundary layer and any metallic and/or ceramic backing material that might be present.

The interface condition (at  $i = I1$ ) can be specified by either of two procedures (see Appendix B):

1. Criteria of continuous flux at the boundary

$$-k1 \left( \frac{\partial T}{\partial x} \right) = -k2 \left( \frac{\partial T}{\partial x} \right). \quad (4)$$

2. Criteria of continuous flux and an operable PDE at the boundary.

In using the code, large time steps should be avoided since they can cause inaccuracies as well as instabilities because of the pulsed boundary condition and the interface between materials 1 and 2. At least 10 time steps for each pulse comprise the upper limit, i.e., for a 10 ms ( $10^{-3}$  s) pulse  $\Delta t$  would be 1 ms. Since the rest period is usually much longer than the pulse period, e.g., 90 ms compared to 10 ms, a larger  $\Delta t$  could be used during this period if conserving computation time became important.

### IV. PRELIMINARY RESULTS AND DISCUSSION

The main purpose of this section is to discuss preliminary results which demonstrate the feasibility of applying our heat transfer model to CTR applications.

#### A. Choice of a test system

A niobium (Nb) - alumina ( $Al_2O_3$ ) radial composite was selected since it is currently under

consideration as a first wall composite material,<sup>3</sup> and because its thermal properties are representative of typical metallic conductors and ceramic insulators that might be considered at a later time. Present Z-pinch design estimates will require an insulating capacity between 1 to 3 kV/cm which will control the relative dimensions of insulator (2) to conductor (1).<sup>2</sup> Although actual sizes have not been specified for a real operating system, a prototype experimental design utilizing anodized aluminum washers (0.0254 cm thick Al with approximately 0.0005 cm of anodized coating) is currently under construction by Phillips and associates.<sup>2</sup> A large scale-up from these dimensions is anticipated for future experiments and consequently a test geometry with about 1 cm width of conductor to 0.1 cm of insulator with an overall wall thickness of 1 cm was selected. Total heat flux loads on the first wall during the pulse period are expected to be the range of 0.1 to 10 kW/cm<sup>2</sup> consisting mainly of Bremsstrahlung and  $n$ - $\gamma$  energy. Niobium, due to its high mass number, will absorb most of the plasma energy within a very thin layer ( $\sim 0.01$ mm).<sup>3</sup> Alumina, on the other hand, will absorb the energy continuously with a distribution function given in Fig. 4. As suggested by Burnett et al.<sup>3</sup> an average electron temperature of 25 keV was selected to define the heat generation function. During the rest period, approximately 10% of the instantaneous pulse heat flux will impinge on the inside surface of the wall with no distribution within the wall ( $H(y) = 0$ ). As a first approximation a constant value was used during the entire rest period (see Fig. 3). In order to meet the Lawson criterion a 10% duty cycle corresponding to a 0.01 s pulse and a 0.09 s rest period has been employed for the test case. A range of outside surface ( $y = Y_{wall}$ , Fig. 2) heat transfer coefficients from  $h = 0.14$  to 14 cal/cm<sup>2</sup> s K were utilized to approximate the thermal resistance anticipated from a niobium (Nb)/boron nitride (BN) protective liner and a molten lithium boundary layer. Average values for material properties were selected at approximately 800°C, and these are tabulated in Table I for several first wall material possibilities.

A summary of the system parameters investigated is presented in Table II. Again, we would like to emphasize that our purpose at this stage was to

TABLE I  
MATERIAL PROPERTIES (\*)

	$k$	$\rho$	$C_p$	$\alpha = k/\rho C_p$
	cal/(cm <sup>2</sup> s K/cm)	g/cm <sup>3</sup>	cal/gK	cm <sup>2</sup> /s
<b>Conductors (1)</b>				
Niobium, Nb	0.158	8.57	0.0736	0.250
Molybdenum, Mo	0.350	10.20	0.0630	0.545
<b>Insulators (2)</b>				
Alumina, $\alpha$ -Al <sub>2</sub> O <sub>3</sub>	0.034	3.96	0.198	0.0434
Beryllia, BeO	0.835	3.00	0.50	0.0557
$k$ -thermal conductivity	$\rho$ -density	$C_p$ -heat capacity	$\alpha$ -thermal diffusivity	

(\*) Data based on information taken at ~800°C from

1. "Perry's Handbook for Chemical Engineers," 4th Ed., McGraw-Hill N.Y., (1965).
2. "Handbook of Chemistry and Physics," Chemical Rubber Publ., N.Y., 41st Ed. (1962).
3. "Thermal Physical Properties of Matter," Vols. 1-2 Eds. Touloukian, Powell, Ho, and Klemens, Plenum Publ. Corp., N.Y. (1970).

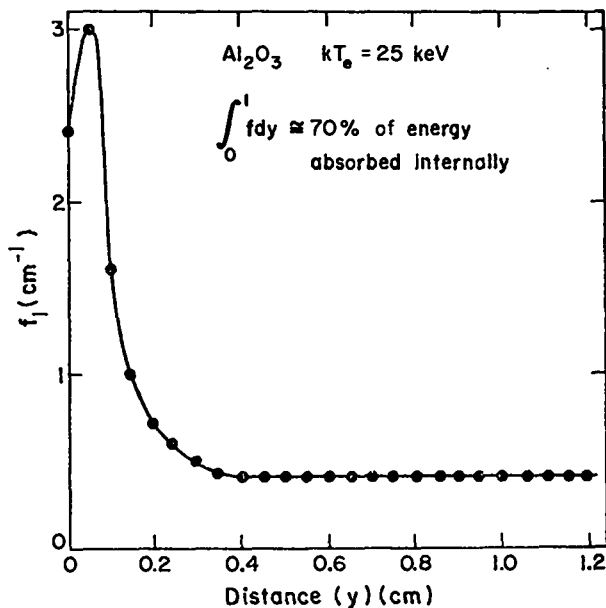


Fig. 4. Heat distribution function for Al<sub>2</sub>O<sub>3</sub> for pulse period (original data Ref 3  $kT_e$ -electron temperature of the plasma).

demonstrate calculational feasibility rather than propose a definitive design.

#### B. Temperature-Time Excursions for a Nb/Al<sub>2</sub>O<sub>3</sub> Composite

Table III (A and B) provides a complete summary of the test runs made. The effects of heat flux, heat transfer coefficient, time step, and grid size parameters were all examined.

A typical temperature-time excursion for seven consecutive pulses (for complete parameter specification see Table III, Run 1) is presented in Fig. 5. Several features of the graph are apparent.

1. There are no inherent instabilities in the ADI solution.
2. The outside surface temperatures,  $\Delta T(0,J)$ ,  $\Delta T(I1,J)$ , and  $\Delta T(I2,J)$ , do not increase due to the large value of  $h = 14 \text{ cal/cm}^2 \text{ s K}$  used.
3. The interface  $\Delta T(I1,0)$  is between the maximum excursion in the Al<sub>2</sub>O<sub>3</sub> layer ( $\Delta T(0,0)$ ) and the minimum in Nb layer ( $\Delta T(0,0)$ ).
4. The inside surface temperature for either material Nb or Al<sub>2</sub>O<sub>3</sub> does not relax to what its initial level was before the pulse, hence there is a continuous increase in  $\Delta T$  which should approach steady-state conditions after a temperature profile of sufficient magnitude has been established

TABLE II  
SYSTEM PARAMETERS INVESTIGATED

1. Duty cycle	$\tau_p = .01 \text{ s}$	$\tau_r = .09 \text{ s}$
2. Incident heat flux		
$q_i$ (pulse period)	0.1-1.0 kw/cm <sup>2</sup>	(-23.82 - 238.2 cal/cm <sup>2</sup> s)
$q_i$ (rest period)	.01-.1 kw/cm <sup>2</sup>	(-2.382 - 23.82 cal/cm <sup>2</sup> s)
3. Heat distribution/generation function H(y)	separate functions for insulator (2) and conductor (1) during pulse and rest mode utilized	
4. Heat transfer coefficient h	.14-14 cal/cm <sup>2</sup> s K outside surface-combined resistance of backing material and liquid lithium	
5. Bulk temperature $T_B$	$= 600^\circ\text{C}^a$	
6. geometrical parameters	wall thickness $Y_{wall} = 1 \text{ cm}$ conductor thickness $L1 = .01-1 \text{ cm}$ Composite insulator thickness $L2 = .0005 - .1 \text{ cm}$	
7. Equation solution parameters	grid sizes $\Delta x1 = .0005 - .05 \text{ cm}$ $\Delta x2 = .0005 - .005 \text{ cm}$ $\Delta y = .01 - .02 \text{ cm}$ time steps $\Delta t = 10 - 2000 \mu\text{s} \quad (10^{-6} \text{ s})$	

<sup>a</sup>Really arbitrary, material limitations will set the upper bound.

to conduct away the total energy deposited during the pulse and rest periods.

A series of temperature profiles are presented in Fig. 6 for the conditions of Run 5 (Table III). In this case, heat was deposited on the inside surface of the Nb layer during both pulse and rest periods and on the inside surface of the Al<sub>2</sub>O<sub>3</sub> layer during the rest period. The heat distribution function given in Fig. 4 was used for Al<sub>2</sub>O<sub>3</sub> during the pulse period. One can see a marked reduction in the temperature excursion of the Al<sub>2</sub>O<sub>3</sub> layer caused by distributing the heat. All three profiles, at the center lines of materials 1 and 2 and the interface, are uniform in shape and magnitude for the

three times given. This effect is also illustrated by comparing Fig. 7b with Fig. 8 which have identical conditions, except in Fig. 8 no heat distribution was used ( $H(y)'s = 0$ ).

The magnitude of the outside surface effective heat transfer coefficient has a significant effect on predicted temperature-time excursions (see Figs. 7a and 7b). With  $h = 0.14 \text{ cal/cm}^2 \text{ s K}$  to approximate anticipated thermal resistances, the outside wall temperature has increased by > 60K over the bulk lithium value in 30 pulses. This  $\Delta T$  will, of course, continue to increase until steady-state conditions are reached.



TABLE III  
TABLE III (SECTION A)  
SUMMARY OF RESULTS FOR COMPOSITE/PULSED CASE<sup>a</sup>

Run	Conductor (1)	Insulator (2)	Geometry			Grid Size			Time Step $\Delta t$	Heat Transfer Coeff. Outside Surface $h$	Total Incident Flux	
			L1	L2	Ywall	$\Delta x1$	$\Delta x2$	$\Delta y$			$q_i$ Rest Period	$q_i$ Pulse Period
			cm	cm	cm	cm	cm	cm			$\mu s$	cal/cm <sup>2</sup> s K
1	Niobium Nb	Alumina Al <sub>2</sub> O <sub>3</sub>	1.0	0.1	1.0	0.05	0.005	0.02	1000	14	0.01	1.0
2	Nb	Al <sub>2</sub> O <sub>3</sub>	0.01	0.0005	1.0	0.0005	0.00005	0.02	1000	14	0.01	1.0
3	Nb	Al <sub>2</sub> O <sub>3</sub>	1.0	0.1	1.0	0.05	0.005	0.02	1000	14	0.01	1.0
4	Nb	Al <sub>2</sub> O <sub>3</sub>	1.0	0.1	1.0	0.05	0.005	0.02	1000	14	0.1	1.0
5+9	Nb	Al <sub>2</sub> O <sub>3</sub>	1.0	0.1	1.0	0.05	0.005	0.02	1000	0.14	0.1	1.0
6	Nb	Al <sub>2</sub> O <sub>3</sub>	1.0	0.1	1.0	0.05	0.005	0.02	100	0.14	0.1	1.0
7	Nb	Al <sub>2</sub> O <sub>3</sub>	1.0	0.1	1.0	0.025	0.0025	0.01	200	0.14	0.1	1.0
8+10	Nb	Al <sub>2</sub> O <sub>3</sub>	1.0	0.1	1.0	0.05	0.005	0.02	1000	0.14	0.1	1.0
	Molybdenum Mo	Beryllia BeO	1.0	0.1	1.0	0.05	0.005	0.02	1000	0.14	0.1	1.0

<sup>a</sup> Conditions fixed for all runs:  $\tau_p = 0.01$  s  $\tau_r = 0.09$  s.

TABLE III (SECTION B)  
SUMMARY OF RESULTS FOR COMPOSITE/PULSED CASE<sup>a</sup>

Run	Heat Distribution Functions Utilized <sup>c</sup>				Steady State Temperature Excursions $\Delta T(x, y, t = \infty)$ <sup>b</sup>				Comments
	Conductor (1) Pulse Period	Conductor (1) Rest Period	Insulator (2) Pulse Period	Insulator (2) Rest Period	Inside Surface (Plasma Side) Conductor $\Delta T(x=0, y=0, t=\infty)$	Interface $\Delta T(x=I1, y=0, t=\infty)$	Insulator $\Delta T(x=I2, y=0, t=\infty)$	Outside Surface Average $\Delta T(\langle x \rangle, y=Ywall, t=\infty)$	
	Hpl(y)	Hrl(y)	Hp2(y)	Hp2(y)	K	K	K	K	
1	0	0	0	0	370	460	490	- 0	
2	0	0	0	0	260	260	260	- 0	unidirectional (y only)
3	0	0	0	0	250	320	380	- 0	
4	0	0	Hp2(y)	0	360	351	348	- 0	
5+9	0	0	Hp2(y)	0	650	640	640	300	
6	0	0	Hp2(y)	0	650	640	640	300 <sup>d</sup>	
7	0	0	Hp2(y)	0	650	640	640	300 <sup>d</sup>	
8+10	0	0	0	0	600	695	810	300	
	0	0	Hp2(y)	0					

<sup>a</sup> Refer to nomenclature section (Appendix F) and Figs. 1-2.

<sup>b</sup> Extrapolated to  $\infty$  time.

<sup>c</sup> Refer to section IIC and Figs. 3-4.

<sup>d</sup> Equivalent to run 5.

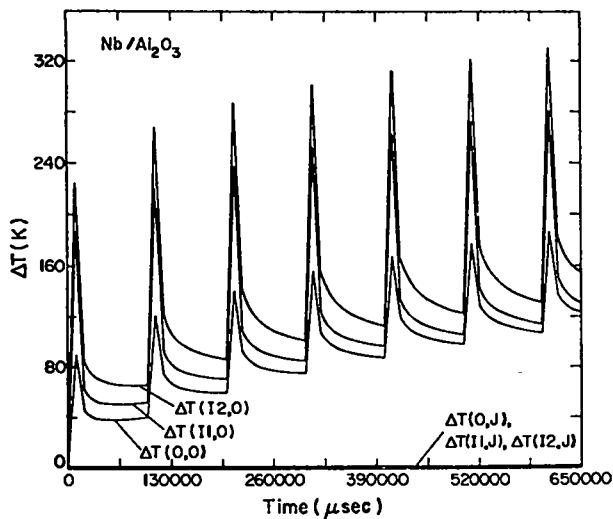


Fig. 5. Temperature-time excursions for a Nb (1cm)/Al<sub>2</sub>O<sub>3</sub> (0.1 cm) composite at six locations. For parameter specifications see Table III, Run 1, and see Fig. 2 for geometrical grid locations.

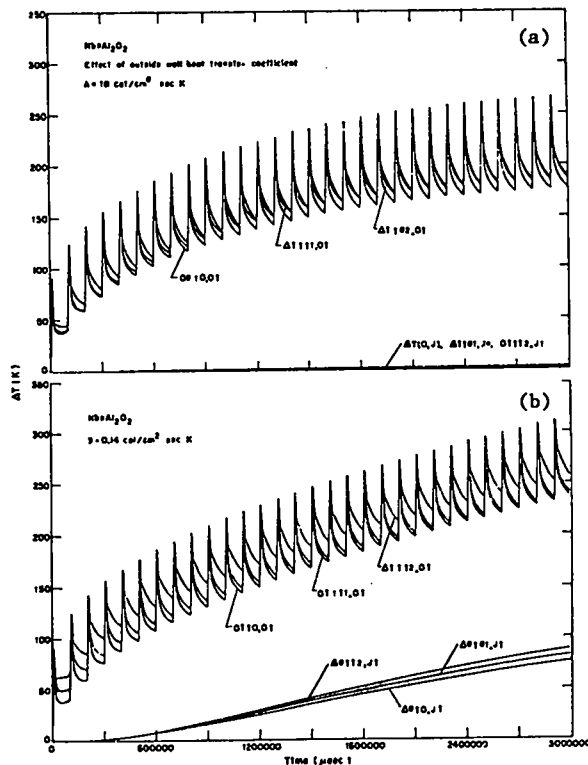


Fig. 7. Effect of outside wall heat transfer coefficient  $h$  on temperature-time excursion for a Nb/Al<sub>2</sub>O<sub>3</sub> composite. For parameter specifications see Table III, Runs 4(7a), 5(7b).

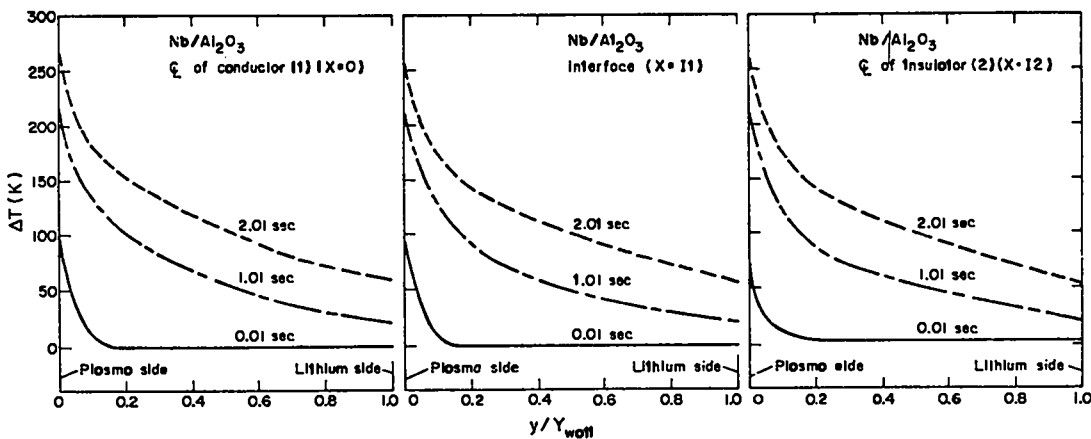


Fig. 6. Approximate temperature profiles  $T = f(y)$  at various times (2.01 s - 21 pulses, 1.01 s - 11 pulses, 0.01 s - 1 pulse). For parameter specifications see Table III, Run 5 and see Fig. 7b for temperature-time excursion.

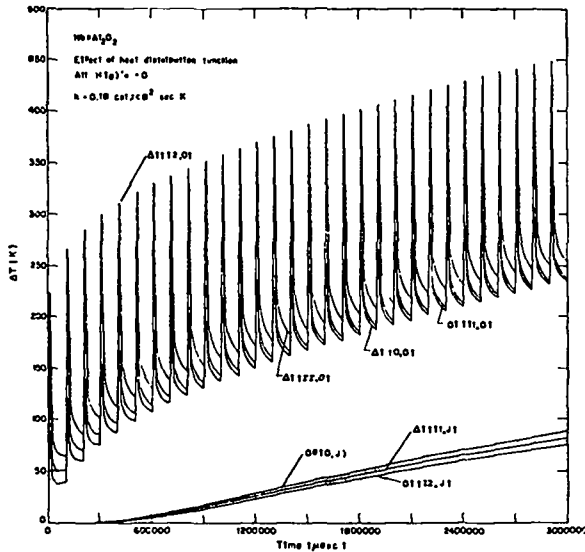


Fig. 8 Effect of heat distribution function on the temperature-time excursion of an Nb/Al<sub>2</sub>O<sub>3</sub> composite. For parameter specifications see Table III, Run 8.

### C. Approach to Steady State

As steady state is reached, the temperature profile at any position along the composite will stabilize except in the vicinity of the inside surface where it is continuously pulsed. This behavior was observed in a preliminary study of heat transfer effects.<sup>1</sup> Because the thermal time constant  $\tau_w = Y_w^2/\alpha$  is large compared to a cycle time of 0.1 s, e.g., for a 1-cm wall  $\tau_w$  (Al<sub>2</sub>O<sub>3</sub>)  $\cong$  23 s and  $\tau_w$  (Nb)  $\cong$  6 s and because an additional thermal resistance is imposed by the low  $h = .14$  cal/cm<sup>2</sup> s K on the outside surface, successive pulsing will cause  $\Delta T$  to increase at any point in the wall. A crude estimate of the maximum  $\Delta T$  anticipated is given by superimposing both the  $\Delta T_a$  equivalent to steady-state heat transfer through the wall and the  $\Delta T_h$  caused by thermal contact resistance at the outside surface onto the  $\Delta T_p$  caused by the pulse itself. For instance, at the center line of the conductor (0,0), an estimate of  $\Delta T_{0,0}^\infty$  at steady state is given by,

$$\Delta T_{0,0}^\infty \cong \Delta T_a + \Delta T_h + \Delta T_p$$

$$\text{where } \Delta T_a = \frac{(\text{net heat transferred/time})}{kl/Y_w}$$

$$= \frac{(q_p \tau_p + q_r \tau_r) Y_w}{(\tau_p + \tau_r) kl}$$

$\Delta T_p$  = temperature rise after the 1st pulse at (0,0)

$$\Delta T_h = \frac{(\text{net heat transferred/time})}{h}$$

$$= \frac{(q_p \tau_p + q_r \tau_r)}{(\tau_p + \tau_r) h}$$

For the case of a 1 kW/cm<sup>2</sup> (238.2 cal/s cm<sup>2</sup>) pulse and a .1 kW/cm<sup>2</sup> (23.82 cal/s cm<sup>2</sup>) heat dump,

$$\Delta T_a = 287 \text{ K}$$

$$\Delta T_p \cong 90 \text{ K}$$

$$\Delta T_h = 333 \text{ K}$$

Therefore,

$$\Delta T_{0,0}^\infty \cong 710 \text{ K}$$

From Table III, one can see that excursions of 650 K are typical for these conditions (Runs 5,6, and 7).

### D. Prototype Geometry - Effective Unidirectional Heat Transport

Run 2 attempted to simulate conditions similar to those expected in the prototype Z-pinch reactor (Fig. 1). The widths of Nb and Al<sub>2</sub>O<sub>3</sub> in the x-direction, .01 cm for Nb and .0005 cm for Al<sub>2</sub>O<sub>3</sub>, are very small compared to the thickness of the wall in the y-direction, 1 cm. Consequently, conduction in the x-direction is fast and can be neglected relative to that in the y-direction and the code performs a unidirectional ADI solution to the PDE using area average properties. In Fig. 9, temperature-time excursions are presented for the case with  $h = 14$  cal/cm<sup>2</sup> s K.

### E. Convergence and Stability of the Method - Effect of Grid Size and Time Step

Convergence of the ADI technique was checked with Runs 6 and 7 by reducing the grid sizes,  $\Delta x_1$  from .05 to .025 cm and  $\Delta x_2$  from .005 to .0025 cm and  $\Delta y$  from .02 to .01 cm, and time step  $\Delta t$  from

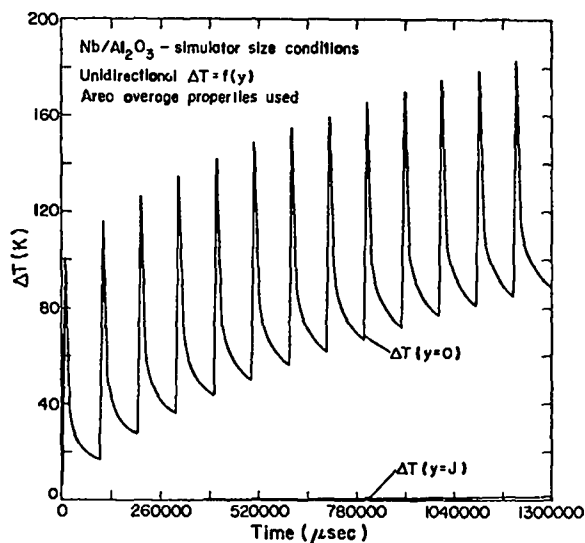


Fig. 9 Temperature-time excursion for a Nb/Al<sub>2</sub>O<sub>3</sub> composite having similar dimensions to the prototype Z-pinch (Fig. 1). For parameter specifications see Table III, Run 2.

1000 to 200  $\mu$  s. Temperature profiles varied by no more than 5% at equivalent grid locations. Furthermore, when the composite was reduced to a single component, e.g., Nb, and a two-dimensional ADI solution was run, x-direction variation of  $\Delta T$  was less than 0.1% and the temperature-time excursions were consistent with previous data accumulated for unidirectional heat flow using an explicit method.<sup>1</sup>

Although the ADI technique, as applied to rectangular two-dimensional problems, should be unconditionally stable regardless of the choices of  $\Delta t$ ,  $\Delta x$ , and  $\Delta y$ ,<sup>9</sup> our specific application of the ADI technique did result in instabilities as mentioned in Sec. III. The pulsed heat flux and interface condition were probably responsible for this since when they were removed from the problem by using a single component and continuous flux boundary,  $\Delta t$

could be selected independently of  $\Delta x$  and  $\Delta y$ . Certain improvements to the stability of the ADI procedure are obtained if the grid system is converted to a half-interval system with the interface containing  $\Delta x/2$  and  $\Delta x/2$  parts of materials 1 and 2.

#### F. Concluding Remarks

The computer model for heat flow in radial composite CTR first wall materials should provide a useful tool for establishing temperature excursions and profiles which are necessary in evaluating the mechanical and chemical behavior of any proposed materials.

#### V. RECOMMENDATIONS

1. Additional materials should be examined, including, ZrO<sub>2</sub>, BeO, and other insulating oxides as well as Ta, Zr, Mo, and other conducting metals.
2. Having established anticipated temperature-time excursions, other properties such as chemical stability, radiation damage including void and helium bubble growth, thermal stressing, and other aspects of materials compatibility should be considered.<sup>1,5,6</sup>
3. By selecting a range of thermal properties, dimensions, incident fluxes, and heat distribution functions, generalized thermal history charts applicable to pulsed-high-beta machines could easily be generated for use in preliminary design work.

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APPENDIX A

FINITE DIFFERENCE EQUATION FORMALISM

Tables A-1 and A-2 list the difference equations utilized by the code. Both sequences of sweeping x first and then y, and vice versa, are presented. In addition, two different equations applying at the interface between materials 1 and 2 are included. A complete description of the nomenclature employed is given in Appendix F and a partial one below for Tables A-1 and A-2. Tridiagonal matrix coefficients are easily determined by recalling that a would be the coefficient of the i-1 term, b the i term, and c the i + 1 term and d the remaining terms. (See Appendix D.)

Nomenclature for Tables A-1 and A-2

$$A1 = \alpha 1 \Delta t / (\Delta x1)^2 - \text{material 1}$$

$$A2 = \alpha 2 \Delta t / (\Delta x2)^2 - \text{material 2}$$

$$B1 = \alpha 1 \Delta t / (\Delta y)^2 - \text{material 1}$$

$$B2 = \alpha 1 \Delta t / (\Delta y)^2 - \text{material 2}$$

$$C1 = H1 / \rho 1 C_{p1} T_B = \text{heat distribution function } (f(y)) \text{ for material 1}$$

$$C2 = H2 / \rho 2 C_{p2} T_B = \text{heat distribution function } (g(y)) \text{ for material 2}$$

$$E = \frac{k2 \Delta x2}{k1 \Delta x1}$$

$$F = [k2 \Delta x1 / k1 \Delta x2]$$

$$G = \frac{k2 \Delta x2 \alpha 1}{k1 \Delta x1 \alpha 2}$$

$$\phi = \left[ C1 + \left( \frac{k2 \Delta x2 \alpha 1}{k1 \Delta x1 \alpha 2} \right) C2 \right] / \left[ 1 + \frac{k2 \Delta x2 \alpha 1}{k1 \Delta x1 \alpha 2} \right]$$

$$\xi = \alpha 1 \left[ 1 + \frac{k2 \Delta x2}{k1 \Delta x1} \right] / \left[ 1 + \frac{k2 \Delta x2 \alpha 1}{k1 \Delta x1 \alpha 2} \right]$$

$$\delta u_{yy} = u_{11,j-1} - 2u_{11,j} + u_{11,j+1}$$

APPENDIX B

FINITE DIFFERENCE EQUATIONS APPLYING AS BOUNDARY CONDITIONS AT THE INTERFACE BETWEEN MATERIALS 1 AND 2

I. CONTINUOUS FLUX AND TEMPERATURE AT THE INTERFACE

Both temperature and heat flux must be continuous at an interface assumed to be in good thermal contact. Using the nomenclature adopted in this report, this is equivalent to saying that

(1)  $u_{11}^*$  is continuous

and

(2) 
$$k1 \frac{(u_{11,j}^* - u_{11-1,j}^*)}{\Delta x1} =$$

$$k2 \frac{(u_{11+1,j}^* - u_{11,j}^*)}{\Delta x2} \quad (8)$$

Equation (8) can be used directly in the tridiagonal matrix since only the terms  $u_{11-1,j}^*$ ,  $u_{11,j}^*$ ,  $u_{11+1,j}^*$  are involved. Therefore, by rearranging Eq. (8), the coefficients  $a_{11}$ ,  $b_{11}$ ,  $c_{11}$ , and  $d_{11}$  can be specified as:

TABLE A-1  
DIFFERENCE EQUATIONS FOR COMPOSITE (X-FIRST)

Difference Equation	Condition	Range	Comments
<u>begin x-sweep</u>			
1. $u_{1,j}^* = u_{0,j}^*$	left boundary material 1	$j = 1, \dots, J-1$ $i = 1, 2$	Symmetry (no flux)
2. $u_{i,j}^* - u_{i,j} = \frac{A1}{2}(u_{i+1,j}^* - 2u_{i,j}^* + u_{i,j-1}^*)$ $+ \Delta t C1 + \frac{B1}{2}(u_{i,j+1} - 2u_{i,j} + u_{i,j-1})$	material 1	$j = 1, \dots, J-1$ $i = 1, \dots, I1-1$	PDE, implicit x
3a. $(u_{I1,j}^* - u_{I1-1,j}^*) \frac{k1}{\Delta x1} = (u_{I1+1,j}^* - u_{I1,j}^*) \frac{k2}{\Delta x2}$	Interface	$j = 1, \dots, J-1$	a. Cont. flux
3b. $u_{I1,j}^* = u_{I1,j} + \phi \Delta t + \xi u_{yy} \frac{\Delta t}{2\Delta y^2}$ $+ \frac{A1}{2} \frac{(u_{I1-1,j}^* + (1+F)u_{I1,j}^* + (F)u_{I1+1,j}^*)}{2(1+G)}$	Interface	$j = 1, \dots, J-1$ $i = I1$	b. Cont. flux and PDE apply
4. $(u_{i,j}^* - u_{i,j}) = \frac{A2}{2}(u_{i+1,j}^* - 2u_{i,j}^* + u_{i-1,j}^*)$ $+ \Delta t C2 + \frac{B2}{2}(u_{i,j+1} - 2u_{i,j} + u_{i,j-1})$	material 2	$j = 1, \dots, J-1$ $i = I1+1, \dots, I2-1$	PDE, implicit x
5. $u_{I2,j}^* = u_{I2-1,j}^*$	right boundary material 2	$j = 1, \dots, J-1$ $i = I2, I2-1$	symmetry (no flux)
<u>begin y-sweep (no heat source term)</u>			
6. $km(u_{i,1}^{**} - u_{i,0}^{**}) = \Delta y q_m / T_B$	material 1 or 2 $m = 1, 2$	$i = 1, \dots, I1-1,$ $I1 + 1, \dots, I2-1$ $j = 0, 1$	inside boundary (incident fixed heat flux) ( $q^* = q_r$ rest time) ( $q^* = q_p$ pulse time)
7a. $u_{i,j}^{**} - u_{i,j}^* = \frac{Am}{2}(u_{i+1,j}^* - 2u_{i,j}^* + u_{i-1,j}^*) + \frac{Bm}{2}(u_{i,j+1}^* - 2u_{i,j}^* + u_{i,j-1}^*)$	$m = 1, 2$	$i = 1, \dots, I1-1,$ $I1 + 1, \dots, I2-1$ $j = 1, \dots, J$	materials 1 or 2 ex- cluding interface and right & left boundaries.
7b. $u_{I1,j}^{**} = u_{I1,j}^* + \frac{A1}{(1+G)}(u_{I1-1,j}^* - (1+F)u_{I1,j}^* + (F)u_{I1+1,j}^*)$ $+ \frac{EA \Delta t}{2\Delta y^2}(u_{I1,j+1}^{**} - 2u_{I1,j}^{**} + u_{I1,j-1}^{**})$	interface	$i = I1$ $j = 1, \dots, J$	PDE implicit y Applies at interface if Eq. (3b) is used
8. $-km(u_{i,J}^{**} - u_{i,J-1}^{**}) = \Delta y h(u_{i,J}^{**})$	$m = 1, 2$	$i = 1, \dots, I1-1,$ $I1+1, \dots, I2-1$ $j = J-1, J$	outside boundary (temp. dependent flow with liq. metal heat transfer coeff.)

TABLE A-2

## DIFFERENCE EQUATIONS FOR COMPOSITE (Y-FIRST)

Difference equation	Conditions	Range	Comments
<u>begin y-sweep</u>			
1. $km(u_{i,1}^* - u_{i,0}^*) = \Delta y q_m / T_B$	materials 1 or 2 $m=1,2$	$i=1, \dots, I1-1, I1+1, \dots, I2-1$ $j=1,0$	inside boundary (incident fixed heat flux) ( $q^* = q_r$ for rest time) ( $q^* = q_p$ for pulse period)
2a. $u_{i,j}^* = u_{i,j} = \frac{Am}{2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) + \Delta t Cm + \frac{Bm}{2}(u_{i,j+1} - 2u_{i,j}^* + u_{i,j-1}^*)$	$m = 1,2$	$i=1, \dots, I1-1, I1+1, \dots, I2-1$ $j=1, \dots, J$	material 1 or 2 (excluding interface and left boundaries)
2b. $u_{I1,j}^* = u_{I1,j} + \frac{C1 + GC2}{(1+G)} \Delta t + \frac{A1}{(1+G)}(u_{I1-1,j} - (1+F)u_{I1,j} + (F)u_{I1+1,j}) + \frac{EA \Delta t}{2\Delta t^2}(u_{I1,j-1}^* - 2u_{I1,j}^* + u_{I1,j+1}^*)$	interface	$i = I1$	Applies at interface if Eq. (6b) is used
3. $km(u_{i,J}^* - u_{i,J-1}^*) = \Delta y h(u_{i,J}^*)$	$m = 1,2$	$i = 1, \dots, I1-1, I1+1, \dots, I2-1$ $j = J-1, J$	outside boundary (temperature dependent flux with liquid metal heat transfer coeff.)
<u>begin x-sweep (no heat source term)</u>			
4. $u_{i,j}^{**} = u_{i,0}^{**}$	material 1 left boundary	$j = 1, \dots, J-1$ $i = 0,1$	symmetry (no flux)
5. $u_{i,j}^{**} - u_{i,j}^* = \frac{A1}{2}(u_{i+1,j}^{**} - 2u_{i,j}^{**} + u_{i-1,j}^{**}) + \frac{B1}{2}(u_{i,j+1}^{**} - 2u_{i,j}^{**} + u_{i,j-1}^{**})$	material 1	$j = 1, \dots, J-1$ $i = 1, \dots, I1-1$	PDE, implicit x
6a. $(u_{I1,j}^{**} - u_{I1-1,j}^{**}) \frac{k1}{\Delta x1} = (u_{I1+1,j}^{**} - u_{I1,j}^{**}) \frac{k2}{\Delta x2}$	interface	$j = 1, \dots, J-1$ $i = I1$	a. continuous flux
6b. $u_{I1,j}^{**} = u_{I1,j}^* + \frac{\xi \delta u_{yy}^* \Delta t}{2\Delta y^2} + \frac{A1}{2(1+G)}(u_{I1-1,j}^{**} + (1+F)u_{I1,j}^{**} + (F)u_{I1+1,j}^{**})$		$j=1, \dots, J-1$ $i = I1$	b. continuous flux and PDE
7. $u_{i,j}^{**} - u_{i,j}^* = \frac{A2}{2}(u_{i+1,j}^{**} - 2u_{i,j}^{**} + u_{i-1,j}^{**}) + \frac{B2}{2}(u_{i,j+1}^{**} - 2u_{i,j}^{**} + u_{i,j-1}^{**})$	material 2	$j = 1, \dots, J-1$ $i = I1+1, \dots, I2-1$	PDE, implicit x
8. $u_{I2,j}^{**} = u_{I2-1,j}^{**}$	material 2 right boundary	$j = 1, \dots, J-1$ $i = I2-1, I2$	symmetry (no flux)

$$\begin{aligned}
a_{11} &= -1 \\
b_{11} &= 1 + \frac{k_2 \Delta x_1}{k_1 \Delta x_2} \\
c_{11} &= -\frac{k_2 \Delta x_1}{k_1 \Delta x_2} \\
d_{11} &= 0
\end{aligned} \tag{9}$$

The stability and convergence of the ADI procedure appeared to depend on the choice of  $\Delta x_1$  and  $\Delta x_2$  for a given  $k_1$  and  $k_2$ . If values of  $\Delta x_2$  were selected such that

$$\frac{k_1}{\Delta x_1} \cong \frac{k_2}{\Delta x_2} \tag{10}$$

the ADI technique was convergent and stable. Consequently, an alternate form of the interface condition was developed to keep the PDE itself continuous at the interface.

## II. CONTINUOUS FLUX AND TEMPERATURE WITH MODIFIED PDE AT THE INTERFACE

By utilizing the technique suggested by Carnahan, Luther, and Wilkes,<sup>7</sup> one can develop appropriate finite difference equations for the boundary between material 1 and 2 for our case. Following the conventions of the model, the dimensionless temperature at position  $11-1$  in material 1 can be approximated by a Taylor expansion as

$$\begin{aligned}
u_{11-1,j} &\cong u_{11,j} - \Delta x_1 \left( \frac{\partial u}{\partial x} \right)_{11^-} \\
&+ \frac{(\Delta x_1)^2}{2} \left( \frac{\partial^2 u}{\partial x^2} \right)_{11^-} + \dots
\end{aligned} \tag{11}$$

by solving Eq. (11) for  $(\partial^2 u / \partial x^2)_{11^-}$ , one gets

$$\begin{aligned}
\left( \frac{\partial^2 u}{\partial x^2} \right)_{11^-} &\cong \frac{2}{(\Delta x_1)^2} \left[ u_{11-1,j} - u_{11,j} \right. \\
&\left. + \Delta x_1 \left( \frac{\partial u}{\partial x} \right)_{11^-} \right]
\end{aligned} \tag{12}$$

Using the finite difference equation for  $(\partial^2 u / \partial y^2)$  and  $\partial u / \partial t$

$$(\partial^2 u / \partial y^2) \cong \frac{1}{\Delta y^2} \left[ u_{11,j+1} - 2u_{11,j} + u_{11,j-1} \right] \tag{13}$$

$$\begin{aligned}
(\partial u / \partial t) &\cong \frac{1}{\Delta t} \left[ u_{11,j}^* - u_{11,j} \right] \\
&u^* \text{ at new time } t + \Delta t
\end{aligned} \tag{14}$$

Likewise for material 2, Eqs. (11), (12), (13), and (14) can be rewritten as,

$$\begin{aligned}
u_{11+1,j} &\cong u_{11,j} + \Delta x_2 \left( \frac{\partial u}{\partial x} \right)_{11^+} \\
&+ \frac{(\Delta x_2)^2}{2} \left( \frac{\partial^2 u}{\partial x^2} \right)_{11^+}
\end{aligned} \tag{15}$$

$$\begin{aligned}
\left( \frac{\partial^2 u}{\partial x^2} \right)_{11^+} &\cong \frac{2}{(\Delta x_2)^2} \left[ u_{11+1,j} - u_{11,j} \right. \\
&\left. - \Delta x_2 \left( \frac{\partial u}{\partial x} \right)_{11^+} \right]
\end{aligned} \tag{16}$$

$$\left( \frac{\partial^2 u}{\partial y^2} \right) \cong \frac{1}{\Delta y^2} \left[ u_{11,j+1} - 2u_{11,j} + u_{11,j-1} \right] \tag{17}$$

$$\left( \frac{\partial u}{\partial t} \right) = \frac{1}{\Delta t} \left( u_{11,j}^* - u_{11,j} \right) \tag{18}$$

By substituting into the differential equation,

$$\alpha \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + c = \frac{\partial u}{\partial t}$$

one can develop an expression for  $\partial u / \partial t$  at the interface. For medium 1, using Eqs. (12), (13), and (14)

$$\begin{aligned}
\alpha_1 &\left[ \frac{2}{(\Delta x_1)^2} \left( u_{11-1,j} - u_{11,j} + \Delta x_1 \left( \frac{\partial u}{\partial x} \right)_{11^-} \right) \right. \\
&+ \frac{1}{\Delta y^2} \left( u_{11,j+1} - 2u_{11,j} + u_{11,j-1} \right) \left. \right] + c_1 \\
&= \left( u_{11,j}^* - u_{11,j} \right) / \Delta t
\end{aligned} \tag{19}$$



Solving for  $(\partial u / \partial x)_{II}^-$ , by defining

$$\delta u_{yy} \equiv u_{II,j-1} - 2u_{II,j} + u_{II,j+1}$$

Eq. (19) becomes

$$\begin{aligned} \Delta x_1 \left( \frac{\partial u}{\partial x} \right)_{II}^- &= \frac{(\Delta x_1)^2}{2\alpha_1 \Delta t} (u_{II,j}^* - u_{II,j}) \\ &- \frac{(\Delta x_1)^2 C_1}{2\alpha_1} - \frac{(\Delta x_1)^2}{2(\Delta y)^2} \delta u_{yy} \\ &+ u_{II,j} - u_{II-1,j} \end{aligned} \quad (20)$$

Similarly for medium 2, using Eqs. (16), (17), and (18)

$$\begin{aligned} -\Delta x_2 \left( \frac{\partial u}{\partial x} \right)_{II}^+ &= \frac{(\Delta x_2)^2}{2\alpha_2 \Delta t} (u_{II,j}^* - u_{II,j}) \\ &- \frac{(\Delta x_2)^2}{2\alpha_2} C_2 - \frac{(\Delta x_2)^2}{2(\Delta y)^2} \delta u_{yy} \\ &+ u_{II,j} - u_{II+1,j} \end{aligned} \quad (21)$$

Applying the interface condition of continuous flux, viz,

$$k_1 \left( \frac{\partial u}{\partial x} \right)_{II}^- = k_2 \left( \frac{\partial u}{\partial x} \right)_{II}^+ \quad (22)$$

We can use Eqs. (20), (21), and (22) to eliminate  $\left( \frac{\partial u}{\partial x} \right)_{II}^-$  and  $\left( \frac{\partial u}{\partial x} \right)_{II}^+$  by just rearranging Eqs. (20 and (21).

$$\begin{aligned} k_1 \left( \frac{\partial u}{\partial x} \right)_{II}^- &= \frac{k_1 \Delta x_1}{2\alpha_1 \Delta t} (u_{II,j}^* - u_{II,j}) \\ &- \frac{k_1 \Delta x_1 C_1}{2\alpha_1} - \frac{k_1 \Delta x_1}{2(\Delta y)^2} \delta u_{yy} \\ &+ \frac{k_1}{\Delta x_1} (u_{II,j} - u_{II-1,j}) \end{aligned} \quad (23)$$

$$\begin{aligned} k_2 \left( \frac{\partial u}{\partial x} \right)_{II}^+ &= -\frac{k_2 \Delta x_2}{2\alpha_2 \Delta t} (u_{II,j}^* - u_{II,j}) \\ &+ \frac{k_2 \Delta x_2 C_2}{2\alpha_2} + \frac{k_2 \Delta x_2}{2(\Delta y)^2} \delta u_{yy} \\ &- \frac{k_2}{\Delta x_2} (u_{II,j} - u_{II+1,j}) \end{aligned} \quad (24)$$

Equations (23) and (24) can be used to solve for  $u_{II,j}^*$ .

$$\begin{aligned} &\left[ \frac{k_1 \Delta x_1}{2\alpha_1 \Delta t} + \frac{k_2 \Delta x_2}{2\alpha_2 \Delta t} \right] u_{II,j}^* \\ &= \left[ \frac{k_1 \Delta x_1}{2\alpha_1 \Delta t} + \frac{k_2 \Delta x_2}{2\alpha_2 \Delta t} \right] u_{II,j} \\ &+ \left[ \frac{k_1 \Delta x_1 C_1}{2\alpha_1} + \frac{k_2 \Delta x_2 C_2}{2\alpha_2} \right] \\ &+ \left[ \frac{k_1 \Delta x_1}{2(\Delta y)^2} + \frac{k_2 \Delta x_2}{2(\Delta y)^2} \right] \delta u_{yy} \\ &- \frac{k_1}{\Delta x_1} [u_{II,j} - u_{II-1,j}] \\ &- \frac{k_2}{\Delta x_2} [u_{II,j} - u_{II+1,j}] \end{aligned} \quad (25)$$

By simplifying Eq. (25),

$$u_{II,j}^* = u_{II,j} + \phi \Delta t + \frac{\xi \Delta t \delta u_{yy}}{\Delta y^2} + \frac{u_{II-1,j} - u_{II,j} \left[ 1 + \frac{k_2 \Delta x_1}{k_1 \Delta x_2} \right] + u_{II+1,j} \left[ \frac{k_2 \Delta x_1}{k_1 \Delta x_2} \right]}{\frac{(\Delta x_1)^2}{2\alpha_1 \Delta t} \left[ 1 + \frac{k_2 \Delta x_2}{k_1 \Delta x_1} \frac{\alpha_1}{\alpha_2} \right]} \quad (26)$$

where

$$\phi \equiv \left[ C1 + \frac{k2\Delta x2 \alpha1}{k1\Delta x1 \alpha2} C2 \right] / \left[ 1 + \frac{k2\Delta x2 \alpha1}{k1\Delta x1 \alpha2} \right] \quad (27)$$

$$\xi = \alpha1 \left[ 1 + \frac{k2\Delta x2}{k1\Delta x1} \right] / \left[ 1 + \frac{k2\Delta x2 \alpha1}{k1\Delta x1 \alpha2} \right] \quad (28)$$

Equation (26) is similar to the explicit difference equation presented by Arpacı.<sup>2</sup>

For the case of no heat generation,  $C1 = C2 = 0$ ;  $\Delta x1 = \Delta x2 = \Delta x$ ; and only one direction dependence for  $u$ , i.e.,  $\delta u_{yy} = 0$ ,  $u^*$  becomes

$$u^*_{II,j} = u_{II,j} + \frac{2\alpha1\Delta t}{\Delta x^2} \left[ u_{II-1,j} - u_{II,j} \left( 1 + \frac{k2}{k1} \right) + u_{II+1,j} \left( \frac{k2}{k1} \right) \right] / \left[ 1 + \frac{k2\alpha1}{k1\alpha2} \right] \quad (29)$$

By multiplying the numerator and denominator of the second term on the right-hand side of Eq. (29) by  $k1/k2$  and rearranging, one gets,

$$u^*_{II,j} = u_{II,j} + \frac{2\alpha1\Delta t}{\Delta x^2} \left[ u_{II+1,j} - u_{II,j} \left( 1 + \frac{k1}{k2} \right) + u_{II-1,j} \left( \frac{k1}{k2} \right) \right] / \left[ \frac{k1}{k2} + \frac{\alpha1}{\alpha2} \right] \quad (30)$$

which corresponds to Eq. (7.67) presented by Carnahan et al.<sup>7</sup> on page 463. If both materials are the same,  $\alpha1 = \alpha2 = \alpha$ ;  $k1 = k2 = k$  and,

$$u^*_{II,j} = u_{II,j} + \frac{\alpha\Delta t}{\Delta x^2} \left( u_{II+1,j} - 2u_{II,j} + u_{II-1,j} \right), \quad (31)$$

which is in standard explicit form for a homogeneous system.

Using implicit formulation in order to implement this algorithm in the current ADI code, one can show that

$$u^*_{II,j} = u_{II,j} + \phi^* \Delta t + \frac{\delta u_{yy} (\Delta t/2) \xi^*}{\Delta y^2} + \frac{\alpha1\Delta t/2}{(\Delta x1)^2} \left[ u^*_{II-1,j} - u^*_{II,j} \left( 1 + \frac{k2\Delta x1}{k1\Delta x2} \right) + u^*_{II+1,j} \left( \frac{k2\Delta x1}{k1\Delta x2} \right) \right] / \left[ 1 + \frac{k2\Delta x2 \alpha1}{k1\Delta x1 \alpha2} \right] \quad (32)$$

with  $\phi = \phi^*$ ,  $\xi = \xi^*$ .

(Note that again the heat source  $\phi^*$  is put in with full  $\Delta t$ , and  $\Delta t/2$  is used for other time intervals.)

To determine the coefficients for the tridiagonal matrix, viz.,  $a_{II}$ ,  $b_{II}$ ,  $c_{II}$ ,  $d_{II}$ , we define the following quantities.

$$E \equiv \frac{k2\Delta x2}{k1\Delta x1}; \quad F \equiv \frac{k2\Delta x1}{k1\Delta x2}; \quad G \equiv \frac{k2\Delta x2 \alpha1}{k1\Delta x1 \alpha2} \quad (33)$$

Note that  $\delta u_{yy} = u_{II,j-1} - 2u_{II,j} + u_{II,j+1}$  is defined at the old time  $t$  rather than  $t + \Delta t$ .

The first three terms on the right-hand side of Eq. (32) are used to specify  $d_{II}$ , while the fourth term specifies  $a_{II}$ ,  $b_{II}$ , and  $c_{II}$ , along with the left-hand side of Eq. (32). Consequently,

$$a_{II} = \frac{-2\alpha1\Delta t/2}{(\Delta x1)^2 (1 + G)} \quad (34)$$

$$b_{II} = 1 + \frac{2\alpha1\Delta t/2 (1 + F)}{(\Delta x1)^2 (1 + G)} \quad (35)$$

$$c_{II} = \frac{-2\alpha1\Delta t/2 (F)}{(\Delta x1)^2 (1 + G)} \quad (36)$$

$$d_{I1} = u_{I1,j} + \frac{\Delta t (C1 + GC2)}{(1 + G)} + \frac{\Delta t \alpha 1 (1 + E)}{2(1 + G) \Delta y^2} [u_{I1,j-1} - 2u_{I1,j} + u_{I1,j+1}] \quad (37)$$

(in the Madcap code  $\alpha 1 = D1$  and  $\alpha 2 = D2$ ).

In the ADI scheme, we also need an equation to allow us to implicitly calculate  $u_{I1,j}$  at the interface when sweeping in the y-direction. Since Eq. (25) is an equivalent form of the PDE applying at  $i = I1$  (interface), it can be rewritten implicit in y and explicit in x. Equation (26) thus can be restructured as

$$u_{I1,j}^* = u_{I1,j} + \phi \Delta t + \frac{\xi \Delta t}{2 \Delta y^2} [u_{I1,j-1}^* - 2u_{I1,j}^* + u_{I1,j+1}^*] + \frac{2\alpha 1 \Delta t / 2}{(\Delta x 1)^2} \left[ \frac{u_{I1-1,j} - u_{I1,j} \left[ 1 + \frac{k2 \Delta x 1}{k1 \Delta x 2} \right] + u_{I1+1,j} \left[ \frac{k2 \Delta x 1}{k1 \Delta x 2} \right]}{\left[ 1 + \frac{k2 \Delta x 2 \alpha 1}{k1 \Delta x 1 \alpha 2} \right]} \right] \quad (38)$$

which is similar to Eq. (32). Again we can solve for the tridiagonal coefficients using Eq. (33) to define terms.

$$u_{I1,j}^* = u_{I1,j} + \frac{\Delta t [C1 + GC2]}{(1 + G)} + \frac{\Delta t \alpha 1}{(\Delta x 1)^2 (1 + G)} [u_{I1-1,j} - (1 + F) u_{I1,j} + (F) u_{I1+1,j}] + \frac{\xi \Delta t}{2 \Delta y^2} [u_{I1,j-1}^* - 2u_{I1,j}^* + u_{I1,j+1}^*] \quad (39)$$

$$\xi = \frac{\alpha 1 (1 + E)}{(1 + G)} \quad (40)$$

$$a_{I1} = \frac{\xi \Delta t}{2 \Delta y^2} = - \frac{\alpha 1 (1 + E) \Delta t}{(1 + G) (2 \Delta y^2)} \quad (41)$$

$$b_{I1} = 1 + \frac{\xi \Delta t}{\Delta y^2} = 1 + \frac{\alpha 1 (1 + E) \Delta t}{(1 + G) \Delta y^2} \quad (42)$$

$$c_{I1} = - \frac{\xi \Delta t}{2 \Delta y^2} = - \frac{\alpha 1 (1 + E) \Delta t}{(1 + G) (2 \Delta y^2)} \quad (43)$$

$$d_{I1} = \frac{\Delta t \alpha 1}{(\Delta x 1)^2 (1 + G)} [u_{I1-1,j} - (1 + F) u_{I1,j} + (F) u_{I1+1,j}] + u_{I1,j} + \frac{\Delta t (C1 + GC2)}{(1 + G)} \quad (44)$$

APPENDIX C

ALTERNATING DIRECTION IMPLICIT METHOD (ADI)

The implementation of the ADI method as discussed in Appendix A has been considered by numerous authors (7,9,10,11), and consequently only a brief discussion is included here. The ADI technique when applied to a rectangular grid network avoids the step size limitations of an explicit method and also uses a tridiagonal coefficient matrix for rapid calculation of the temperature grid at any time step. The basic concept is to use two difference equations, each applied at half  $\Delta t$  steps.

Each difference equation is implicit in either the x or y direction. For example, solving the two-dimensional elliptic equation

$$\alpha \left[ \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right] = \frac{\partial u}{\partial t} \quad (45)$$

would involve iterations using difference equations of the following form for an (i,j) grid. The x-sweep [implicit in x] is written as

$$\frac{u_{i,j}^* - u_{i,j}}{\Delta t/2} = \frac{(u_{i-1,j}^* - 2u_{i,j}^* + u_{i+1,j}^*)}{\Delta x^2} + \frac{(u_{i,j-1} - 2u_{i,j} + u_{i,j+1})}{\Delta y^2}, \quad (46)$$

and the y-sweep [implicit in y] as

$$\frac{u_{i,j}^{**} - u_{i,j}^*}{\Delta t/2} = \frac{(u_{i-1,j}^* - 2u_{i,j}^* + u_{i+1,j}^*)}{\Delta x^2} + \frac{(u_{i,j-1}^{**} - 2u_{i,j}^{**} + u_{i,j+1}^{**})}{\Delta y^2}, \quad (47)$$

where

$u_{i,j}$  = value of  $u_{i,j}$  at time t

$u_{i,j}^*$  = value of  $u_{i,j}$  at  $t + \Delta t/2$  (half time step)

$u_{i,j}^{**}$  = value of  $u_{i,j}$  at  $t + \Delta t$  (full time step).

Richtmyer and Morton<sup>3</sup> have demonstrated that this form of the ADI method is unconditionally stable regardless of the choice of  $\Delta x$ ,  $\Delta y$ , or  $\Delta t$ . Our particular problem has three additional complications:

- (1) A heat source term C is present [Eq. (1)].
- (2) An interface between two materials is present.
- (3) The inside boundary condition is time dependent (pulsed flux).

All of the above can induce instabilities and/or inadequate convergence unless the difference equations applying at the interface and boundaries are properly formulated. (See Appendix B.) Consistency for the difference equations has been demonstrated if the heat source term is introduced at the full time step, i.e.,  $C\Delta t$  is introduced in either the x

or y sweep and not at both half-time steps.<sup>5</sup> Systematic errors due to this procedure were eliminated by altering the sweeping sequence to  $xyxyxyx \dots$

APPENDIX D

FORMULATION OF THE TRIDIAGONAL ALGORITHM

The ADI technique inherently generates equations for each grid point involving 3 adjacent terms in the u matrix.

$$u_{i-1,j}, u_{i,j}, u_{i+1,j}$$

or

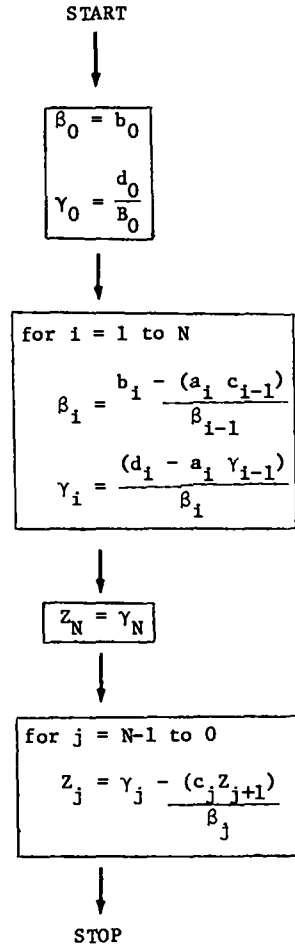
$$u_{i,j-1}, u_{i,j}, u_{i,j+1} \quad (48)$$

The coefficients a,b,c refer to i-1 (j-1), i(j), and i+1(j+1) terms, respectively, while d refers to the remaining terms. Furthermore the a,b,c coefficients would be for terms involving the new time step either u\* or u\*\* (see Table I). Thus, the tridiagonal matrix can be represented as

$$\begin{bmatrix} b_0 z_0 & c_0 z_1 & & & \\ a_1 z_0 & b_1 z_1 & c_1 z_2 & & \\ & \dots & \dots & \dots & \\ & & a_i z_{i-1} & b_i z_i & c_i z_{i+1} \\ & & & \dots & \dots \\ & & & & a_n z_{n-1} & b_n z_n \end{bmatrix} = \begin{bmatrix} d_0 \\ d_1 \\ \dots \\ d_i \\ \dots \\ d_n \end{bmatrix} \quad (49)$$

[Z] refers either to  $u_{i,j}$ , j fixed, or  $u_{i,j}$ , i fixed. The algorithm for solving the tridiagonal matrix is relatively straightforward. The matrix is swept from top to bottom and then from bottom to top to solve for [Z]. The following flow sheet depicts this procedure.<sup>7</sup>

TRIDIAGONAL PROCEDURE



## APPENDIX E

## MADCAP V LISTING

26 Jul 73 0926+11

Rec 01 Page 01

01,001		'CTM COMPOSITE HEAT FLUX MODEL'
01,002		'ALTERNATING DIRECTION IMPLICIT METHOD USED'
01,003		'Pulsed case'
01,004		'Isotropic and homogeneous properties assumed for each material'
01,005		'Modified Code with continuous interface condition'
01,006		'Variable Specification'
01,007		'T = temperature, °C'
01,008		'T <sub>B</sub> = bulk lithium temperature, °C'
01,009		'Cp = heat capacity, cal/g°C'
01,00a		'p = density, g/cm <sup>3</sup> '
01,00b		'h = heat transfer coefficient, cal/cm <sup>2</sup> sec°C'
01,00c		'k = thermal conductivity, cal/cm sec°C'
01,00d		'D = thermal diffusivity = k/ρC <sub>p</sub> , cm <sup>2</sup> /sec'
01,00e		'Tp = burn time for pulse, Micro-sec'
01,00f		'Tr = test time, Micro-sec'
01,010		'Δx1 = x-step size in Material 1'
01,011		'Δx2 = x-step size in Material 2'
01,012		'Δy = y-step size'
01,013		'Δt = step size for time'
01,014		'Time = actual time, sec'
01,015		'Tprint = interval between prints micro-sec'
01,016		'Y <sub>w</sub> = wall thickness, cm'
01,017		'L1 = size of material 1 element, cm'
01,018		'L2 = size of material 2 element, cm'
01,019		'sub or postscripts 1 and 2 refer to two different materials'
01,01a		'sub or postscript 3 refers to average value at interface'

01,01b | | | | | | | | | | | | | |  
"Differential Equation (Rectangular coordinates)"  
01,01c "Differential Equation (Rectangular coordinates)"  
$$D(d^2u/dx^2 + d^2u/dy^2) + C(y) = du/dt$$
  
01,01d "Dimensionless parameters"  
01,01e " $u = (T - T_B)/T_B$ "  
01,01f " $A = \Delta t / \Delta x^2$ "  
01,020 " $B = \Delta t / \Delta y^2$ "  
01,021 " $Cat = \Delta t / \rho C_p$ "  
01,022 " $Q_{ay}/R = \text{incident heat flux}$ "  
01,023 "where:"  
01,024 "Postscripts 1 and 2 refer to two different materials"  
01,025 "postscripts r and p refer to rest and burn periods"  
01,026 "For example,"  
01,027 "H is the internal heat generation term, it can take on"  
01,028 "values:  $Hr1(y), Hp1(y), Hr2(y), Hp2(y)$ "  
01,029 "Likewise for Q:  $Qr1, Qp1, Qr2, Qp2$ "  
01,02a " $u_e = \text{dimensionless temperature at } 1/2 \text{ time step}$ "  
01,02b " $u_{ee} = \text{dimensionless temperature at complete time step}$ "

```

02,001      | | | | | | | | | |
'sense 1 - on for trial data set'
02,002      'sense 2 - on for print out at each'
02,003      'sense 3 - on set generation terms to zero'
02,004      'sense 4 - on to set up plots'
02,005      'sense 5 - on to terminate the iteration'
02,006      'sense 6 - on to terminate iteration and initial plotting'
02,007      'sense 7 - on ask for new print interval'
02,008      'sense 8 - on to use old interface condition at I1'
02,009      '      -K1(du/dx) = -K2(du/dx) in finite difference form'
02,00a      '      off to use modified interface condition at I1'
02,00b      '      Continuous flux and PDE apply'
02,00c      'if cont. flux and PDE are used at the interface then the'
02,00d      'interface is included in the y sweep'
02,00e      'sense 9 - on to use harmonic mean for interface,'
02,00f      '      off for arithmetic area average'
02,010      u,u*,u**0 to 110,0 to 110
02,011      Z,a,b,c,d0 to 110
02,012      Gr1,Gr2,Op1,Op2,Hr1,Hr2,Hp1,Hp20 to 110
02,013      Z,y0 to 110
02,014      'Array assignment for plots'
02,015      'ΔT = T-T1, °C'
02,016      'ΔT1 = inside surface (plasma) temp. rise for material 1 at (i=1,j=0)'
02,017      'ΔT2 = inside surface (plasma) temp. rise for material 2 at (i=I2-1,j=0)'
02,018      'ΔT3 = inside surface (plasma) temp. rise at interface (i=I1,j=0)'
02,019      'ΔT4 = outside surface (lithium) temp. rise for material 1 (i=1,j=J)'
02,01a      'ΔT5 = outside surface (lithium) temp. rise for material 2 (i=I2-1,j=J)'
02,01b      'ΔT6 = outside surface (lithium) temp. rise at interface (i=I1,j=J)'

```



```

02,01c      | | | | | | | | | |
             ΔT1,ΔT2,ΔT3,ΔT4,ΔT5,ΔT6,t0 to 500
02,01d      Ca10 to 2000
02,01e      Yax1a0 to 500
02,01f      D6290 to 10
02,020      w = 0
02,021      t0.ΔT10.ΔT20.ΔT30.ΔT40.ΔT50.ΔT60 = 0
02,022      (200 characters) COMP1,COMP2
02,023      for i = 0 to 110
02,024          ai.bi.ci.di.zi = 0
02,025          ΔT11.ΔT21.ΔT31.ΔT41.ΔT51.ΔT61 = 0
02,026          for j = 0 to 110
02,027              u1,j.u*1,j.u**1,j = 0
02,028      fo is •          Temperature Profiles (T-TB, °C) •

```

```

03,001      I  I  I  I  I  I  I  I  I  I  I  I  I  I  I  I  I  I  I  I  I  I
            I1 is "i = 0 1 1/2 I I I I I I I I I I I I I I I I I I I I I I
03,002      I2 is " j"
03,003      Tstop = 1000000
03,004      if sense 1 is on      "Trial data set"
03,005          read console by " Δt = x ΔX1 = x ΔX2 = x Δy = x " : Δt, ΔX1, ΔX2, Δy
03,006          read console by "L1 = x L2 = x Yval1 = x" : L1, L2, Yv
03,007          read console by " k1 = x k2 = x " : k1, k2
03,008          read console by " Cp1 = x Cp2 = x " : Cp1, Cp2
03,009          read console by " p1 = x p2 = x " : p1, p2
03,00a          read console by " D1 = x D2 = x " : D1, D2
03,00b          read console by " h = x " : h
03,00c          read console by " Qr1 = x Qr2 = x "
03,00d      cont.          " Cp1 = x Cp2 = x " : Qr1, Qr2, Qp1, Qp2
03,00e          read console by " cOMP1 = x cOMP2 = x " : comp1, comp2
03,00f          read console by " Tprint(=micro-sec) = x " : Tprint
03,010      if sense 1 is on
03,011          read console by " Tstop=x " : Tstop
03,012      otherwise          "input data"
03,013          Δt=1000; ΔX1=.05; ΔX2=.005; ΔY=.02
03,014          L1 = 1 ; L2 = .1 ; Yv = 1
03,015          k1=.158; k2=.034
03,016          Cp1=.0731; Cp2=.178
03,017          p1=8.57; p2=3.96
03,018          D1=.25; D2=.0434
03,019          h = .14
03,01a          Qr1 = 23.82 ; Qr2 = 23.82
03,01b          Qp1=238.2; Qp2=238.2
03,01c          Comp1 = "kb"

```

```
03,01d      ( { | | | | | | | | | | | | | | | | )
             Comp2 = *A1_2*sigma_3  small h = .1k cal/cm^2sec^0C *
03,01e             Tprint = 10000
03,01f             Tstop = 3000000
03,020             T_g = 600           *°C*
03,021             T_p = 10000        *micro-sec*
03,022             T_r = 90000        *micro-sec*
03,023             I_p = [(T_p/delta t)]
03,024             I_t = [(T_p + T_r)/delta t]
03,025             I1 = [(L1/(2*delta x1) + .5)]
03,026             I2 = I1 + [(L2/(2*delta x2) + .5)]
03,027             J = [(Y_v/delta y + .5)]
03,028             delta t = .000001 delta t      *conversion to sec from micro sec*
03,029             A1 = D1{delta t/delta x1^2}
03,02a             A2 = D2{delta t/delta x2^2}
03,02b             B1 = D1{delta t/delta y^2}
03,02c             B2 = D2{delta t/delta y^2}
03,02d             if sense 9 is on      *harmonic mean*
03,02e             k3 = [2k1*k2]/(k1+k2)
```

```

04,001      | | | | | | | | | |
otherwise      "arithmetic area average"
04,002      k3 = (k1*Ax1+k2*Ax2)/(Ax1+Ax2)
04,003      Index = 1
04,004      Delta = [(,000001 x Tprint/At + .5)]
04,005      "internal heat generation functions as arrays"
04,006      if sense 3 is off
04,007          read card by "(d10)5": Points,Fract1,Fract2,Fract3,Fract4
04,008          new card
04,009          for i = 0 to Points
04,00a          read card by "(d10)5": y1,Gr1,Gp11,Gr21,Gp21
04,00b          new card
04,00c          Degree = 2
04,00d          i0 = 1
04,00e          for j = 0 to J
04,00f              ȳ = j(Ay)
04,010              for i = i0 to Points
04,011                  if y1 ≥ ȳ
04,012                      execute lagran(j,i,Degree,ȳ)
04,013                      i0 = i
04,014                      exit from loop
04,015                  otherwise: loop back
04,016      otherwise
04,017          Fract1 = 1
04,018          Fract2 = 1
04,019          Fract3 = 1
04,01a          Fract4 = 1
04,01b          for j = 0 to J

```

```

04,01c      |   |   |   |   |   |   |   |   |   |
              Hr1j, Hp1j, Hr2j, Hp2j = 0

04,01d      *Conversion from percent absorption to heat, cal/cm3sec *
04,01e      for j = 0 to J
04,01f          Hr1j = Qr1 * Hr1j / Δy
04,020          Hr2j = Qr2 * Hr2j / Δy
04,021          Hp1j = Qp1 * Hp1j / Δy
04,022          Hp2j = Qp2 * Hp2j / Δy

04,023      Qr1 = Fract1 * Qr1
04,024      Qr2 = Fract2 * Qr2
04,025      Qp1 = Fract3 * Qp1
04,026      Qp2 = Fract4 * Qp2
04,027      for i = 0 to I2          *Initial condition ui,j = 0*
04,028          for j = 0 to J
04,029              ui,j, ui,jn, ui,jn+1 = 0
04,02a      Time = 0
04,02h      *begin. of iterations for each time period Δt as n=1 to infinity*
04,02c      *Code will proceed with one of two algorithms*
04,02d      * 1 - if x and y Profiles are important, 2-D ADI*
04,02e      * is used with entire heat source added at one*
04,02f      * half time step, and iteration sequence altered*
04,030      * as YYYYYYX in sweeping x and y arrays,*
04,031      * 2 - if composite has very small x dimensions,*
04,032      * i.e. if L1 and L2 are small compared to the*
04,033      * thermal diffusion depths, only the y direction*
04,034      * is used in the code, and a unidirectional ADI*
04,035      * is run with average property values used*
04,036      *Test for parabolic (2D) or unidirectional dependence*

```

```

      | | | | | | | | | |
05,001   Twx1 = (L1/2)2/D1
05,002   Twx2 = (L2/2)2/D2
05,003   Twy1 = Yw2/D1
05,004   Twy2 = Yw2/D2
05,005   if sense 8 is off or (k1=k2) and (D1=D2) and (Δx1=Δx2)
05,006       Iomit = I2+1      'includes interface in computation'
05,007   otherwise
05,008       Iomit = I1      'excludes interface'
05,009   for n = 2 to infinity
05,00a       if model() = 1      'Parabolic ADI (2D) x and y Directions'
05,00b           if index ≤ Ip      'Counter to determine if in pulse or rest mode'
05,00c               q1 = Qp1
05,00d               q2 = Qp2
05,00e               q3 = (q1*Δx1+q2*Δx2)/(Δx1+Δx2)
05,00f           otherwise
05,010               q1 = Qr1
05,011               q2 = Qr2
05,012               q3 = (q1*Δx2+q2*Δx2)/(Δx1+Δx2)
05,013           if n is even      'sweep x first'
05,014               execute eqone(i)
05,015           for j = 1 to J-1
05,016               if index ≤ Ip
05,017                   C1 = Hp1j/(p1*cp1*Ts)      'pulse period'
05,018                   C2 = Hp2j/(p2*cp2*Ts)
05,019               otherwise
05,01a                   C1 = Hr1j/(p1*cp1*Ts)      'rest period'

```

```

05,01b      |   |   |   |   |   |   |   |   |
              C2 = Kr2_j / (p2 * Cp2 * T_B)
05,01c      for i = 1 to I1-1
05,01d          execute eqtwo(i,j,A1,B1,C1,At,1)
05,01e      execute eqthree(I1,j,k1,k2,D1,D2,C1,C2,Ax1,Ax2,Ay,At,0)
05,01f      for i = I1+1 to I2-1
05,020          execute eqtwo(i,j,A2,B2,C2,At,1)
05,021      execute eqfive(I2)
05,022      execute std(I2,a,b,c,d,Z)
05,023      for i = 0 to I2
05,024          u*_{i,j} = Z_i
05,025      for i = 1 to I2-1 + i + Iomit          "begin y sweep"
05,026          if i < I1: A=A1;B=B1;k=k1;q=q1          "material 1"
05,027          if i = I1: q=q3; k=k3          "interface"
05,028          if i > I1: A=A2;B=B2;k=k2;q=q2          "material 2"
05,029      execute eqsix(0,Ay,q,k,T_B)
05,02a      for j = 1 to J-1
05,02b          if i + I1
05,02c              execute eqfour(i,j,B,A,0,0,0)
05,02d          otherwise
05,02e              execute eqseven(I1,j,k1,k2,D1,D2,0,0,Ax1,Ax2,Ay,At,0)
05,02f      execute eqeight(j,Ay,b,k)

```

```

06,001      | | | | | | | | | |
              execute std(J,a,b,c,d,Z)
06,002      for J = 0 to J
06,003      u1,j = Zj
06,004      otherwise:      *Sweep y first*
06,005      for i = 1 to I2-1 + i + Iomit
06,006      if i < I1: A=A1;B=B1;k=k1;q=q1      *material 1*
06,007      if i = I1: q=q3;k=k3      *interface*
06,008      if i > I1: A=A2;B=B2;k=k2;q=q2      *material 2*
06,009      execute eqsix(0,Ay,q,k,TB)
06,00a      for j = 1 to J-1
06,00b      if Index ≤ Ip
06,00c      C1 = Hp1j / (p1×Cp1×TB)
06,00d      C2 = Hp2j / (p2×Cp2×TB)
06,00e      otherwise
06,00f      C1 = Hr1j / (p1×Cp1×TB)
06,010      C2 = Hr2j / (p2×Cp2×TB)
06,011      if i < I1: C = C1
06,012      otherwise: C = C2
06,013      if i ≠ I1
06,014      execute eqtwo(i,J,B,A,C,At,0)
06,015      otherwise
06,016      execute eqseven(I1,J,k1,K2,D1,D2,C1,C2,Ax1,Ax2,Ay,At,1)
06,017      execute eqeight(J,Ay,h,k)
06,018      execute std(J,a,b,c,d,Z)
06,019      for J = 0 to J
06,01a      u1,j = Zj
06,01b      for j = 1 to J-1      *begin of x sweep*

```



```

06,01c      | | | | | | | | |
             | | | | | | | | |
             | | | | | | | | |
06,01c      execute eqone(0)
06,01d      for i = 1 to I1-1
06,01e      execute eqfour(1,j,A1,B1,0,0,1)
06,01f      execute eqthree(I1,j,K1,K2,D1,D2,0,0,dx1,dx2,dy,dt,1)
06,020      for i = I1+1 to I2-1
06,021      execute eqfour(1,j,A2,B2,0,0,1)
06,022      execute eqfive(I2)
06,023      execute std(I2,a,b,c,d,Z1)
06,024      for i = 0 to I2
06,025      u**i,j = Zi
06,026      *Missing values for u at (i=0,I1,I2; j=0,J) are assigned via B.C.'s*
06,027      *These are not used in the computation of u(x,y,t)*
06,028      u**0,0 = u**1,0
06,029      u**0,J = u**1,J
06,02a      u**I2,0 = u**I2-1,0
06,02b      u**I2,J = u**I2-1,J
06,02c      if k2 ≠ k1      *interface values at j=0,J*
06,02d      Phi = (k2*dx1)/(k1*dx2)
06,02e      u**1,0 = ((Phi*u**1+1,0 + u**I1-1,0)/(1 + Phi)

```



```

07,01c      ( ( ( ( ( ( ( ( ( ( ( (
              for i = 0 to I2
07,01d          for j = 0 to J
07,01e              ui,j = Zj
07,01f          if Index = It: Index=I
07,020          otherwise: Index=Index+I          *end of At period*
07,021          if sense 2 is on: Interval = 0
07,022          otherwise: Interval = IP
07,023          if (n=-1) = Interval(mod Delta)
07,024                                      *OUTPUT*
07,025          Time = (n+1)At
07,026          if sense k is on          *set up arraye for plotting*
07,027              w = w+1
07,028              tw = Time
07,029              AT1w = u0,0nTB
07,02a              AT2w = uI2,0nTB
07,02b              AT3w = uI1,0nTB
07,02c              AT4w = u0,JnTB
07,02d              AT5w = uI2,JnTB
07,02e              AT6w = uI1,JnTB
07,02f          if [(1000000/Time) = [(Tprint))]
07,030              new page
07,031              print: date
07,032              skip k lines
07,033              print: "CTR COMPOSITE FIRST WALL"
07,034              skip 2 lines
07,035              if mod(1) = 1
07,036                  print: "Two dimensional ADI (x and y)"
07,037              otherwise
07,038                  print: "Unidirectional ADI (y-only)"
07,039                  print: "average property values used"

```

```

08,001      | | 1 | | | | | | | |
              skip 1 line
08,002      print: "heat generation functions for pulse and rest mode"
08,003      for j = 0 to J
08,004      print by "j=xx y_j=x,xh Hr1=x,x5+ee "
08,005 cont.      "Hr2=x,x5+ee Hp1=x,x5+ee "
08,006 cont.      "Hp2=x,x5+ee": j,jx4y,Hr1_j,Hr2_j,Hp1_j,Hp2_j

08,007      new page
08,008      print: date
08,009      skip 4 lines
08,00a      print: "CTR COMPOSITE FIRST WALL"
08,00b      skip 2 lines
08,00c      if model() = 1
08,00d      print: "Two dimensional ADI (x and y)"
08,00e      otherwise
08,00f      print: "Unidirectional ADI (y only)"
08,010      print: "Average property values used"
08,011      skip 1 line
08,012      if sense 8 is on
08,013      print: "cont, flux interface condition"
08,014      otherwise
08,015      print: "cont, flux and PpE at interface"
08,016      if sense 9 is on
08,017      print: "harmonic mean for k at interface"
08,018      otherwise
08,019      print: "arithmetic area average for k at interface"
08,01a      print by "conductor(1) = x      insulator(2) = x":0comp1,Comp2
08,01b      skip 1 line
08,01c      print: "incident flux - k(dT/dy)y = 0"

```

```

08,014      | | | | | | | | | |
              | | | | | | | | | |
print by * pulse period qp1=x1,x1 qp2=x1,x1*

08,01e cont.      *cal/sec cm2: Qp1,Qp2

08,01f      print by * rest period qr1=x1,x1 qr2=x1,x1*

08,020 cont.      *cal/sec cm2: Qr1,Qr2

08,021      skip 1 line

08,022      print by *wall thickness (y direction) = x3,x1 cm*:Yw

08,023      print by *element size material 1 (x direction) = x3,x1 cm*:L1

08,024      print by *element size material 2 (x direction) = x3,x6 cm*:L2

08,025      skip 1 line

08,026      print by *Δt = x5 micro-sec *: [(1000000Δt + .5)]

08,027      print by *Δx1 = x4,x5 cm *:ΔX1

08,028      print by *Δx2 = x4,x5 cm *:ΔX2

08,029      print by *Δy = x4,x5 cm *:ΔY

08,02a      skip 1 line

08,02b      print by *D1Δt/Δx12=x1,x5*: A1

08,02c      print by *D2Δt/Δx22=x1,x5*: A2

08,02d      print by *D1Δt/Δy2=x1,x5*: B1

```

```

09,001      |   |   |   |   |   |   |   |   |   |
              {   {   {   {   {   {   {   {   {   {
09,001      print by 'D2dt/dy2 =x4,x5': B2
09,002      skip 1 line
09,003      print by 'Pulse time = x,x5 sec rest time = x,x5 sec':
09,004 cont.      Tp/1000000,Tr/1000000
09,005      skip 1 line
09,006      print by 'for material 1 k= x3,x5 cal/sec cm0C '
09,007 cont.      'Cp= x3,x5 cal/g0C p= x3,x4 g/cm3 '
09,008 cont.      'D1= x3,x5 cm2/sec': k1,Cp1,p1,D1
09,009      skip 1 line
09,00a      print by 'for material 2 k= x3,x5 cal/sec cm0C '
09,00b cont.      'Cp= x3,x5 cal/g0C p= x3,x4 g/cm3 '
09,00c cont.      'D2= x3,x5 cm2/sec': k2,Cp2,p2,D2
09,00d      skip 2 lines
09,00e      print by ' h = x3,x4 effective heat transfer coeff, cal/cm2sec0C =sh
09,00f      skip 1 line
09,010      print by 'Grid size = (x(material 1) = x3 points, '
09,011 cont.      'x(material 2) = x3 points) by (y = x3 points)'(I1,I2-I1).J
09,012      new page
09,013      print by 'Time= x Micro-sec ': 1000000 Time
09,014      skip 2 lines
09,015      print : f0
09,016      print: f1
09,017      print: f2
09,018      skip 2 lines
09,019      I76 = {(I1/2)}
09,01a      I77 = {(I1,I2)/2}

```

```

09,01b      | | | | | | | | | |
              for j = 0 to J
09,01c      print by "xxx.,(.,xx,x1+e)7.,": j,
09,01d cont.      "0,jNTB,"1,jNTB,"176,jNTB"
09,01e cont.      "11,jNTB,"177,jNTB,"12-1,jNTB"
09,01f cont.      "12,jNTB"
09,020      if sense 7 is on
09,021      read console by "Tprint=x": Tprint
09,022      Delta = ((.000001*NTTprint/AT+5))
09,023      if sense 6 is on
09,024      Tstop = 0
09,025      if 1000000*NTTime > Tstop and sense 4 is on
09,026      "plotting routine"
09,027      for n = 1 to 6
09,028      for j = 1 to w
09,029      if n = 1: Yaxisj = AT1j
09,02a      if n = 2: Yaxisj = AT2j
09,02b      if n = 3: Yaxisj = AT3j
09,02c      if n = 4: Yaxisj = AT4j
09,02d      if n = 5: Yaxisj = AT5j
09,02e      if n = 6: Yaxisj = AT6j
09,02f      D629n = MAXn=1 to w {Yaxisn}
09,030      Tmax = MAXn = 1 to 6 {D629n}

```

```

0a,001      | | | | | | | | | |
3629 = * TIME MICRO-SEC*
0a,002      T629 = * T-Tn (C) *
0a,003      U629 = *COMPOSITE-PULSED CASE*
0a,004      execute cprinc(Ca1,2000,1,12)
0a,005      execute csymbol(,1,9,5,,1k,U629,0)
0a,006      execute csymbol(,1,9,2,,1k,Comp1,0)
0a,007      execute csymbol(,1,9,0,,1k,Comp2,0)
0a,008      if Tmax <500 : Tmax = 500
0a,009      otherwise: Tmax = 1000
0a,00a      Tstop = 1000000*Tmax
0a,00b      execute cscalr(0,Tstop,0,Tmax,0,10.0,10)
0a,00c      execute cplot(0,Tmax,3)
0a,00d      execute cplot(Tstop,Tmax,2)
0a,00e      execute cplot(Tstop,0,2)
0a,00f      execute caxis(0,0,0,10,3629,17)
0a,010      execute caxis(0,0,90,-10,T629,-10)
0a,011      for n = 1 to 6
0a,012          symb = n
0a,013          for m = 0 to v
0a,014              if n = 1: Yaxism = ΔT1m
0a,015              if n = 2: Yaxism = ΔT2m
0a,016              if n = 3: Yaxism = ΔT3m
0a,017              if n = 4: Yaxism = ΔT4m
0a,018              if n = 5: Yaxism = ΔT5m
0a,019              if n = 6: Yaxism = ΔT6m
0a,01a          q629 = 3
0a,01b          for n = 0 to v

```



```

0a,01c      ( | | | | | | | | | | | | |
              execute cplot(1000000tm,Yaxism,q629)
0a,01d      q629 = 2
0a,01e      execute cnumb((Tstop+.02),Yaxisy,11,Symb,0,0)
0a,01f      execute cempty(1,1)
0a,020      stop #1
0a,021      if sense 5 is on, stop
0a,022      'Procedures'
0a,023      'eooone thru eoeight generate coefficients for the tridiagonal matrix'
0a,024      ' eooone - left hand boundary-material 1 (x-direction)'
0a,025      ' eotwo - material 1 or 2, PDE at even  $\Delta t/2$ '
0a,026      ' eqthree - interface condition at I1 (x-direction)'
0a,027      ' eofour - material 1 or 2, PDE at odd  $\Delta t/2$ '
0a,028      ' eqfive - right hand boundary-material 2 (x-direction)'
0a,029      ' eosix - inside(D1,asKa) side boundary (y-direction)'
0a,02a      ' eqseven - interface condition (PDE) for y sweep'
0a,02b      ' eoeight - outside, liquid metal heat transfer coeff, (y direction)'
0a,02c      'std solves the tridiagonal matrix'
0a,02d      'lagran generates a lagrangian interpolation polynomial for'
0a,02e      'estimating discrete values of the heat generation term'
    
```

```

Ob,001      |   |   |   |   |   |   |   |   |
             *Model() determines with a 2-D or unidirectional solution*
Ob,002      *will be used*
Ob,003      (...  eqone(n,j,all)
Ob,004      a_n=0;b_n=1;c_n=-1;d_n=0
Ob,005      ...)
Ob,006      (...  eqtwo(n,m,r,s,C,At,Test,j,all)
Ob,007      {array}u
Ob,008      if Test = 1
Ob,009          x = (u_{n,m+1} - 2u_{n,m} + u_{n,n-1})
Ob,00a          k* = n
Ob,00b      otherwise
Ob,00c          x = (u_{n+1,m} - 2u_{n,m} + u_{n-1,m})
Ob,00d          k* = n
Ob,00e      a_{k*} = -r/2
Ob,00f      b_{k*} = 1+r
Ob,010      c_{k*} = -r/2
Ob,011      d_{k*} = 0*x*dt + (s/2) (x) + u_{n,x}
Ob,012      ...)
Ob,013      (...  eqthree(I1,j,k1,k2,D1,D2,C1,C2,dx1,dx2,dy,At,Test2,j,all)
Ob,014      {array}{u,u*
Ob,015      if schse 8 is on      *Continuous flux at interface*
Ob,016          a_{I1} = -1
Ob,017          b_{I1} = 1+(k2*dx1)/(k1*dx2)
Ob,018          c_{I1} = -(k2*dx1)/(k1*dx2)
Ob,019          d_{I1} = 0
Ob,01a      otherwise      *continuous flux and PDE apply at interface*

```

```

Ob,01b      |      |      |      |      |      |      |
             E = (k2*Δx2)/(k1*Δx1)
Ob,01c      F = (k2*Δx1)/(k1*Δx2)
Ob,01d      G = (k2*Δx2*Δt)/(k1*Δx1*Δt)
Ob,01e      aI1 = -(D1*Δt)/(Δx12(1+G))
Ob,01f      bI1 = 1 + (D1*Δt(1+F))/(Δx12(1+G))
Ob,020      cI1 = -(D1*Δt*F)/(Δx12(1+G))
Ob,021      if Test2 = 0
Ob,022              H = D1(1+E)(Δt/2)*(uI1,j-1-2uI1,j+uI1,j+1)/(Δy2)
Ob,023              H2 = uI1,j
Ob,024      otherwise
Ob,025              H = D1(1+E)(Δt/2)*(uI1,j-1-2uI1,j+uI1,j+1)/(Δy2)
Ob,026              H2 = uI1,j
Ob,027      dI1 = H2+(Δt(C1+G*C2)+H)/(1+G)
Ob,028      ...
Ob,029      !... eqfour(n,m,r,s,C,Δt,Test2)
Ob,02a      !array)u*
Ob,02b      if Test = 1
Ob,02c              x = (un,n+1-2un,n+un,n-1)
Ob,02d              k* = n
Ob,02e      otherwise
Ob,02f              x = (un+1,n-2un,n+un-1,n)
Ob,030              k* = n
Ob,031      ak* = -r/2
Ob,032      bk* = 1+r

```

```

Ob,033      |   |   |   |   |   |   |   |   |   |
             cke = -r/2
Ob,034      dke = 0*Δt+α(x)/2+un,n
Ob,035      ...
Ob,036      (... eqfive(I2,j,all)
Ob,037      aI2 = -1; bI2 = 1; cI2 = 0; dI2 = 0
Ob,038      ...
Ob,039      (... eqsix(n,Δy,q,k,Tn,j,all)
Ob,03a      an = 0; bn = 1; cn = -1; dn = (q*Δy)/(k*Tn)
    
```

```

Oc,001      ... |   |   |   |   |   |   |   |   |   |
Oc,002      (... eqseven(I1,j,k1,k2,D1,D2,C1,C2,Δx1,Δx2,Δy,Δt,Test3,j,all)
Oc,003      (array)u,u#
Oc,004      K = (k2*Δx2)/(k1*Δx1)
Oc,005      F = (k2*Δx1)/(k1*Δx2)
Oc,006      G = (k2*Δx2*D1)/(k1*Δx1*D2)
Oc,007      H = D1*(1+Σ)/(1+G)
Oc,008      P = (Δt*D1)/(Δx12(1+G))
Oc,009      if Test3 = 1
Oc,00a      K = P(uI1-1,j-1+PuI1,j+FuI1+1,j)
Oc,00b      K2 = uI1,j
Oc,00c      otherwise
Oc,00d      K = P(uI1-1,j-1+PuI1,j+FuI1+1,j)
Oc,00e      K2 = uI1,j
Oc,00f      aI1 = -(K*Δt)/(2Δy2)
Oc,010      bI1 = 1+(K*Δt)/(Δy2)
Oc,011      cI1 = -(K*Δt)/(2Δy2)
Oc,012      dI1 = K2+H+Δt(C1+G*C2)/(1+G)
Oc,013      ...
Oc,014      (... eqeight(n,Δy,h,k,j,all)
Oc,015      an = -1; bn = 1+Δy*h/k; cn = 0; dn = 0
Oc,016      ...
Oc,017      (... std(n,a,b,c,d,Z)          "Tridiagonal matrix algorithm"
Oc,018      (array)a,b,c,d,Z
Oc,019      B,0 to 110
    
```

```

0c,01a      |   |   |   |   |   |   |   |   |
             for n = 0 to 110
0c,01b      Bn0 = 0
0c,01c      B0 = b0
0c,01d      G0 = d0/B0
0c,01e      for n = 1 to n
0c,01f      Bn = bn - ancn-1/Bn-1
0c,020      Gn = (dn - anGn-1)/Bn
0c,021      Zn = Gn
0c,022      for n = n-1, n-2, ..., 0
0c,023      Zn = Gn - cnZn+1/Bn
0c,024      ...
0c,025      i, .. lagran(j, i, Degree, j) A111
0c,026      (array) Hp1, Hp2, Hr1, Hr2, Gp1, Gp2, Gr1, Gr2, x, y
0c,027      for k = 1 to k
0c,028          if k=1: x=Gp1
0c,029          if k=2: x=Gp2
0c,02a          if k=3: a=Gr1
0c,02b          if k=k: a=Gr2
0c,02c          c = 1
0c,02d          for j = i-1 to i+Degree-1
0c,02e              if  $\bar{y} = y_{j^*}$ 
0c,02f                  Hp1j = Gp1j^*
0c,030                  Hp2j = Gp2j^*
0c,031                  Hr1j = Gr1j^*
0c,032                  Hr2j = Gr2j^*
0c,033                  exit from procedure
0c,034                  otherwise: c=c*( $\bar{y}-y_{j^*}$ )
0c,035           $\bar{a} = 0$ 
0c,036          for i = i-1 to i+Degree-1
0c,037              t = c2i / ( $\bar{y} - y_{i^*}$ )
0c,038              for j = i-1 to i+Degree-1
0c,039                  if i = j: loop back
0c,03a                  t = t / (yi - yj^*)
0c,03b           $\bar{a} = \bar{a} + t$ 
0c,03c          if k=1: Hp1j =  $\bar{a}$ 
0c,03d          if k=2: Hp2j =  $\bar{a}$ 

```

```

      I   I   I   I   I   I   I   I   I   I   I
0d,001      if k=3; Hr1j =  $\frac{1}{2}$ 
0d,002      if k=4; Hr2j =  $\frac{1}{2}$ 
0d,003      ...
0d,004      (... model(nones all)
0d,005      Tbarx = (Twx1+Twx2)/2
0d,006      Tbary = (Twy1 + Twy2)/2
0d,007      if Tbarx < .01Tbary
0d,008          model() = 0      'unidirectional'
0d,009      otherwise
0d,00a          model() = 1      '2-dimensional'
0d,00b      ...
$

```

APPENDIX F

NOMENCLATURE

Variable Specification

$A1 = \alpha1 \Delta t / (\Delta x1)^2$   
 $A2 = \alpha2 \Delta t / (\Delta x2)^2$   
 $B1 = \alpha1 \Delta t / (\Delta y)^2$   
 $B2 = \alpha2 \Delta t / (\Delta y)^2$   
 $C1 = H1 / \rho1 C_p 1 T_B$   
 $C2 = H2 / \rho2 C_p 2 T_B$   
 $C_p$  = heat capacity, cal/g°C  
 $C(y) = H(y) / \rho C_p T_B$  designated as C1 or C2  
 $D$  or  $\alpha$  = thermal diffusivity =  $k / \rho C_p$ , cm<sup>2</sup>/s  
 $\Delta y$  = step size in both materials (y direction)  
 $\Delta x1$  = step size in material 1 (x direction)  
 $\Delta x2$  = step size in material 2 (x direction)  
 $\Delta t$  = full time step  
 $\Delta T = T - T_B$  K or °C  
 $F = k2 \Delta x1 / k1 \Delta x2$   
 $h$  = heat transfer coefficient (liquid lithium, cal/cm<sup>2</sup> s °C)  
 $H(y)$  = heat generation rate, cal/s cm<sup>3</sup>, designated as H1, H2, H1, H2

$I1$  = number of grid pts in x-direction material 1  
 $I2$  = number of grid pts in x-direction material 2  
 $J$  = number of grid pts in x-direction material 2  
 $k$  = thermal conductivity, cal/s cm°C  
 $L1$  = size of element in material 1  
 $L2$  = size of element in material 2  
 $\rho$  = density, g/cm<sup>3</sup>  
 $q$  or  $q_i$  = incident flux on the inside surface  
 $T$  = temperature, K or °C  
 $T_B$  = bulk Lithium temp., K or °C  
 $\tau_p$  = burn time for pulse,  $\mu$  s or m s  
 $\tau_r$  = rest time,  $\mu$  s or m s  
 $u$  = dimensionless temperature =  $(T - T_B) / T_B$   
 $u_{i,j}^*$  = dimensionless temp. 1/2 time interval  
 $u_{i,j}^{**}$  = dimensionless temp. full-time interval

Subscripts or postscripts

1-material 1  
 2-material 2  
 r-rest period  
 p-pulse (burn) period

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