EGG-EAST--8557

DE89 016363

METAL-WATER REACTION AND CLADDING DEFORMATION MODELS FOR RELAP5/MOD3

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June 1989

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Prepared for the U.S. Department of Energy
Idhao Operations Office
Under DOE Contract No. DE-AC07-76ID01570

ABSTRACT

A model for calculating the reaction of zirconium with steam according to the Cathcart-Pawel correlation has been incorporated into RELAP5/MOD3. A cladding deformation model which computes swelling and rupture of the cladding according to the empirical correlations of Powers and Meyer has also been incorporated into RELAP5/MOD3. This report gives the background of the models, documents their implementation into the RELAP5 subroutines, and reports the developmental assessment done on the models.

ACKNOWLEDGMENT

This metal-water reaction and cladding deformation models which have been incorporated into RELAP5/MOD3 are derived from similar models which were incorporated into RELAP5/MOD2[1] by Intermountain Technologies Incorporated and the Netherlands Energy Research Foundation. Studsvik Nuclear of Sweden has been the sponsor of the implementation of the models into RELAP5/MOD3 as part of the Swedish contribution to the ICAP code improvement program.

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METAL-WATER REACTION AND CLADDING DEFORMATION MODELS FOR RELAP5/MOD3

1. INTRODUCTION

One of the goals of the RELAP5/MOD3 development project is to extend the capability of RELAP5 so that it can simulate large-break loss-of-coolant accidents. Cladding deformation can be important during a LB-LOCA because plastic strain of a fuel rod's cladding has a direct effect on calculated cladding temperature. The reaction of the zirconium cladding with steam may be important in LB-LOCA simulations as well as other simulations if the cladding's temperatures reach high enough temperatures. The addition of a metal-water reaction model and a cladding deformation model to RELAP5 helps satisfy one of the goals of the RELAP5/MOD3 project.

2. DESCRIPTION OF METAL-WATER REACTION MODEL

The reaction of zirconium and steam is treated using the correlation developed by Cathcart.[2] The metal-water reaction model is coupled with the fuel rod deformation model so that if a rod ruptures the inside of the cladding can react. The model assumes that there is an unlimited amount of steam available for the metal-water reaction.

The chemical equation being modeled is

$$Zr + 2H_2O \rightarrow ZrO_2 + 2H_2 + 5.94E8\ J/(kg\text{-}mole)$$

The oxide layer thickness on the cladding's outer surface at time point n is given by

$$dr_n = sqrt\ [dr^2_{n-1} + K*dt*exp\ (-A/RT)]$$

where,

dr_n	=	thickness at time point n, m
dr_{n-1}	=	thickness at time point n-1, m
K	=	2.252E-6 m^2/s
dt	=	time step size (t_n - t_{n-1}), sec
A	=	35889 mole/cal
R	=	1.987 cal/(K-mole)
T	=	cladding temperature, K.

The amount of heat added to the cladding's outer surface between time point n and n-1 is given multiplying the volume of cladding undergoing reaction by the density of zirconium and the reaction heat release:

$$Q = \rho\pi\ [(r_o - dr_{n-1})^2 - (r_o - dr_n)^2]\ H/W$$

where:

Q = heat addition per unit length, J/m
ρ = density of zirconium, 6500 Kg/m^3
r_o = cladding outer radius, m
H = reaction heat release, 5.94E8 J/(kg-mole)
W = molecular weight of zirconium (91.22), kg/(kg-mole).

Similar equations are used for the cladding's inner surface if cladding rupture occurs.

The total hydrogen mass generated by the metal-water reaction is calculated by multiplying the mass of zirconium reacted by the ratio of the molecular weight of 4 hydrogen atoms to one zirconium atom (4:91.22).

3. DESCRIPTION OF CLADDING DEFORMATION MODEL

An empirical cladding deformation model from FRAP-T6[3] has been incorporated into RELAP5/MOD3. The model may be invoked only in conjunction with the dynamic gap conductance model. The purpose of the model is to allow plastic deformation of the cladding to be accounted for in the calculation of fuel rod's cladding temperature during LOCA simulations; and to inform a user of the possible occurrence of rod rupture and flow blockage and hence the necessity of conducting more detailed simulations of the fuel rods' behavior.

With the deformation model modifications an additional term is included in the gap conductance (Eq 575) of Reference 1) to account for radiation across the gap

$$h_r = F\,(T^2_f + T^2_c)(T_f + T_c)$$

$$F = 1 / \{1/ef + [R_f/R_c][1/(e_c - 1)]\}$$

where,

h_r = radiation gap conductance

= Stefan-Boltzman constant, 5.67E-8 $W/(m^2\ K^4)$

F = emissivity factor

e_f = emissivity of fuel

e_c = emissivity of cladding

R_f = outer radius of fuel, m

R_c = inner radius of cladding, m

T_f = temperature of fuel's outer surface, K

T_c = temperature of claddings inner surface, K.

When the deformation model is active the total cladding strain is the sum of the thermal strain, the elastic strain, and a plastic strain given by

$$E_p = 0.25\ E_{rup} \exp\,[-0.0153(T_r - T_c)]$$

where

E_p	=	plastic hoop strain before rupture
E_{rup}	=	cladding strain at rupture
T_r	=	rupture temperature, C
T_c	=	average cladding temperature, C.

The rupture temperature is

$$T_r = 3960 - [20.4S/(1+H)] - [8.51E6\ S/(100(1+H) + 2790S)]$$

where

S	=	cladding hoop stress (kpsi)
H	=	max [(heating rate)/(28C/s), 1.0]

The rupture temperature correlation is depicted in Figure 1.

Plastic strain is calculated only if the average cladding temperature exceeds T_{plas}, the temperature at which plastic strain begins

$$T_{plas} = \begin{cases} T_r - 70 & ; \quad T_r < 700 \\ T_r - 70 - 0.14*(T_r - 700) & ; \quad 700 < T_r < 1300 \\ T_r - 155 & ; \quad 1300 < T_r \end{cases}$$

If the average cladding temperature exceeds the value of T_{plas} then the rupture temperature is used together with the heating rate to determine the rupture strain E_{rup}, via a table lookup. When rupture occurs a similar table lookup is used to obtain the flow blockage. The rupture strain and blockage tables are from NUREG-0630.[4] The correlations used for cladding strain and rupture are given in Table 1 and illustrated in Figures 2-4.

If a fuel rod ruptures the rod's internal pressure is set equal to the external fluid's pressure; metal-water reaction is initiated on the inner surface of the cladding for the structure where rupture occurs if the

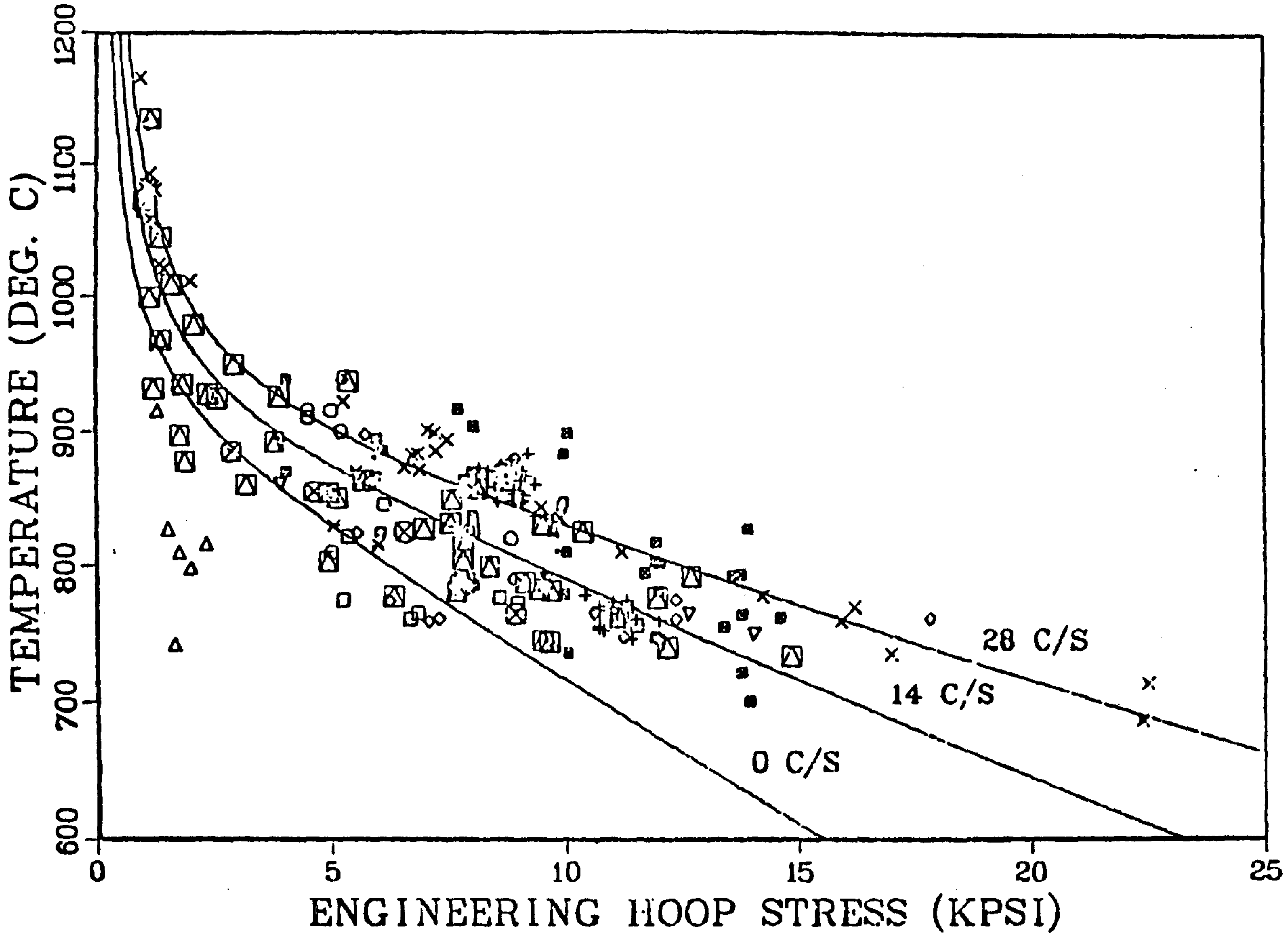

Fig. 1 ORNL correlation of rupture temperature as a function of engineering hoop stress and temperature-ramp rate with data from internally heated Zircaloy cladding in aqueous atmospheres.

TABLE 1. TABULATION OF CLADDING CORRELATIONS

Rupture Temperature (C)	Slow-Ramp Correlations ($\leq$10 C/s) Burst Strain (%)	Slow-Ramp Correlations ($\leq$10 C/s) Flow Blockage (%)	Fast-Ramp Correlations ($\leq$25 C/s) Burst Strain (%)	Fast-Ramp Correlations ($\leq$25 C/s) Flow Blockage (%)
600	10	6.5	10	6.5
625	11	7.0	10	6.5
650	13	8.4	12	7.5
675	20	13.8	15	10.0
700	45	33.5	20	13.8
725	67	52.5	28	20.0
750	82	65.8	38	27.5
775	89	71.0	48	35.7
800	90	71.5	57	43.3
825	89	71.0	60	46.0
850	82	65.8	60	46.0
875	67	52.5	57	43.3
900	48	35.7	45	33.5
925	28	20.0	28	20.0
950	25	18.0	25	18.0
975	28	20.0	28	20.0
1000	33	24.1	35	25.7
1025	35	25.7	48	35.7
1050	33	24.1	77	61.6
1075	25	18.0	80	64.5
1100	14	9.2	77	61.6
1125	11	7.0	39	28.5
1150	10	6.5	26	18.3
1175	10	6.5	26	18.3
1200	10	6.5	36	26.2

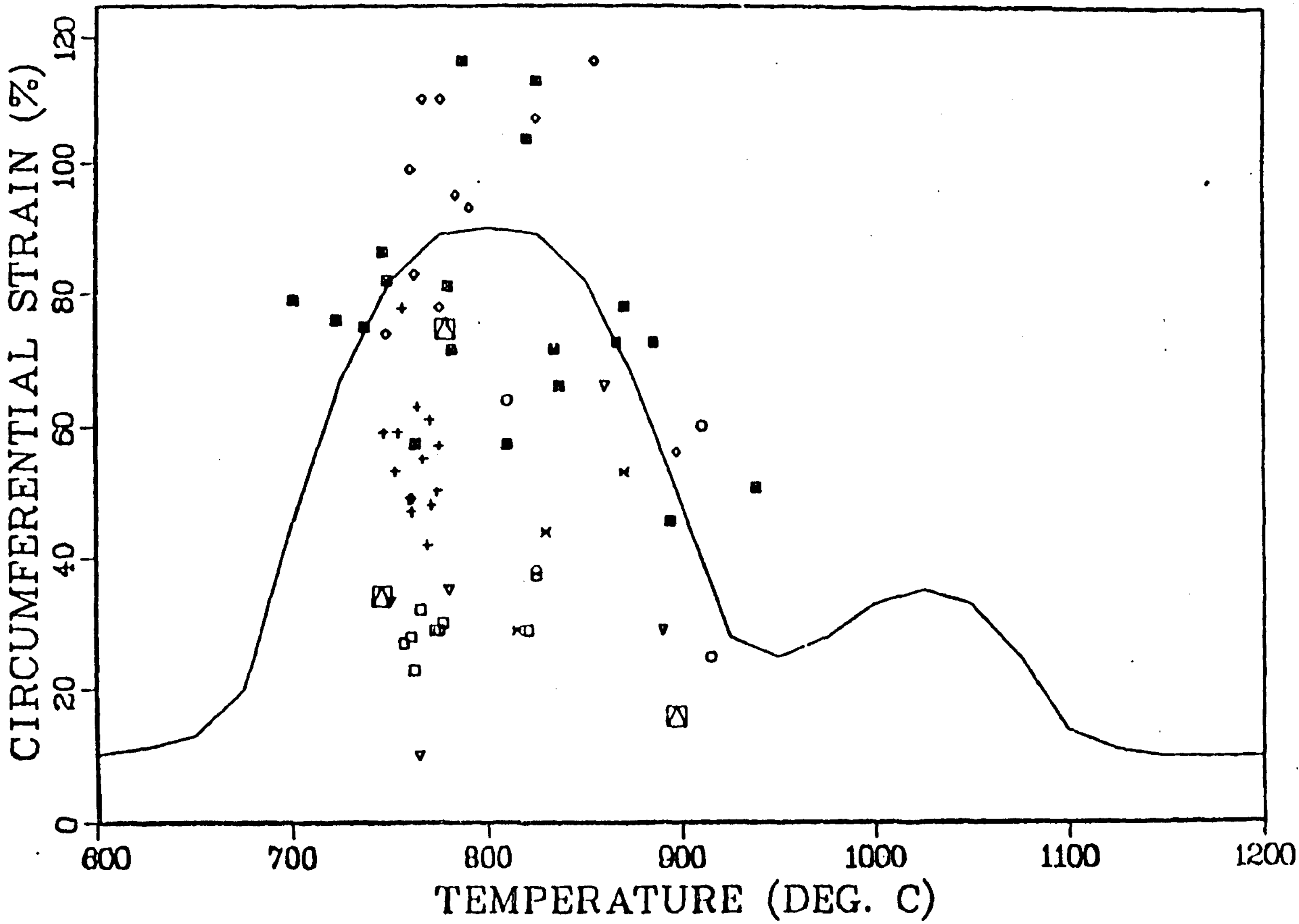

Fig 2 Maximum circumferential strain as a function of rupture temperature for internally heated Zircaloy cladding in aqueous atmospheres at heating rates less than or equal to 10°C/s.

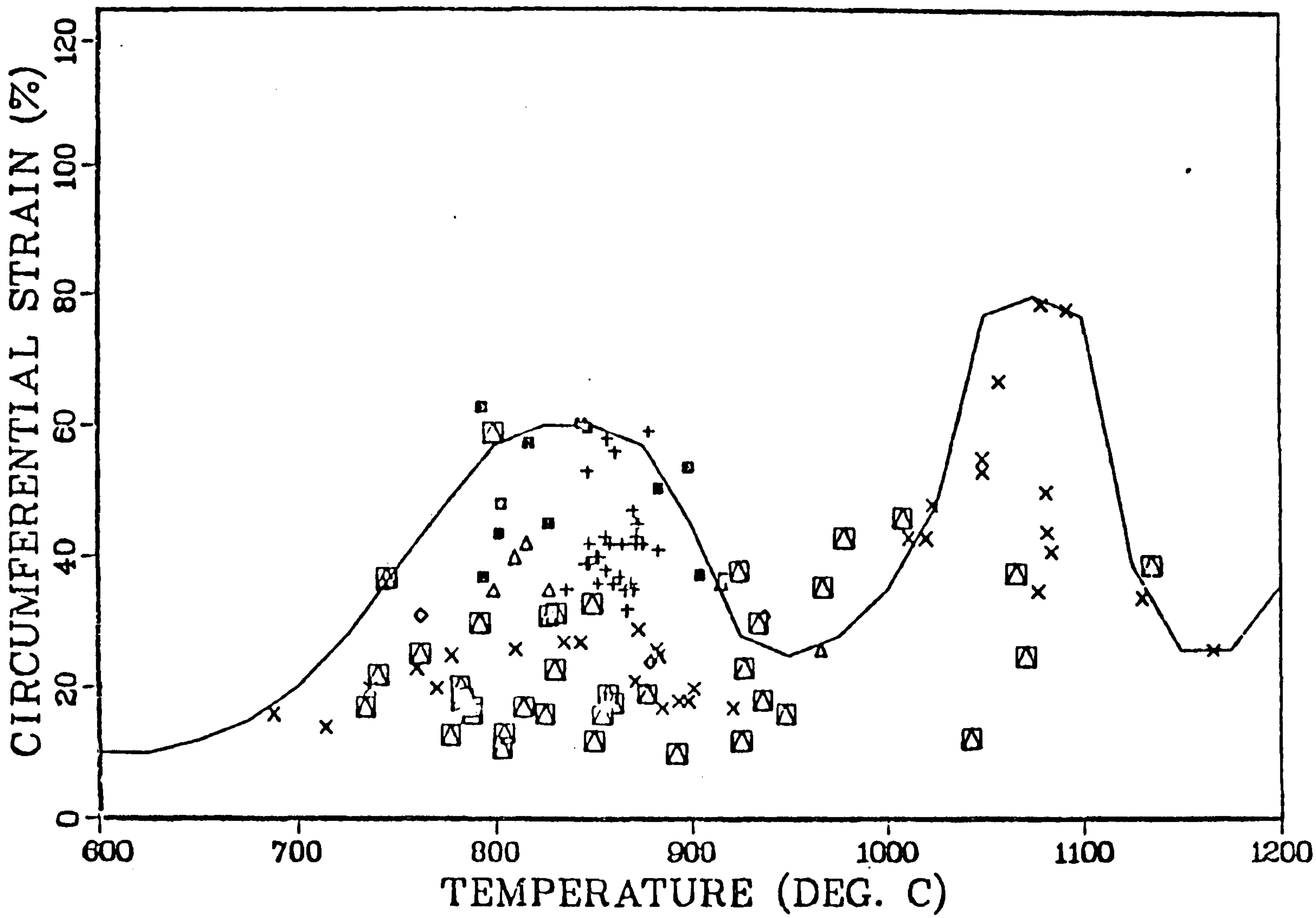

Fig. 3 Maximum circumferential strain as a function of rupture temperature for internally heated Zircaloy cladding in aqueous atmospheres at heating rates greater than or e to 25°C/s.

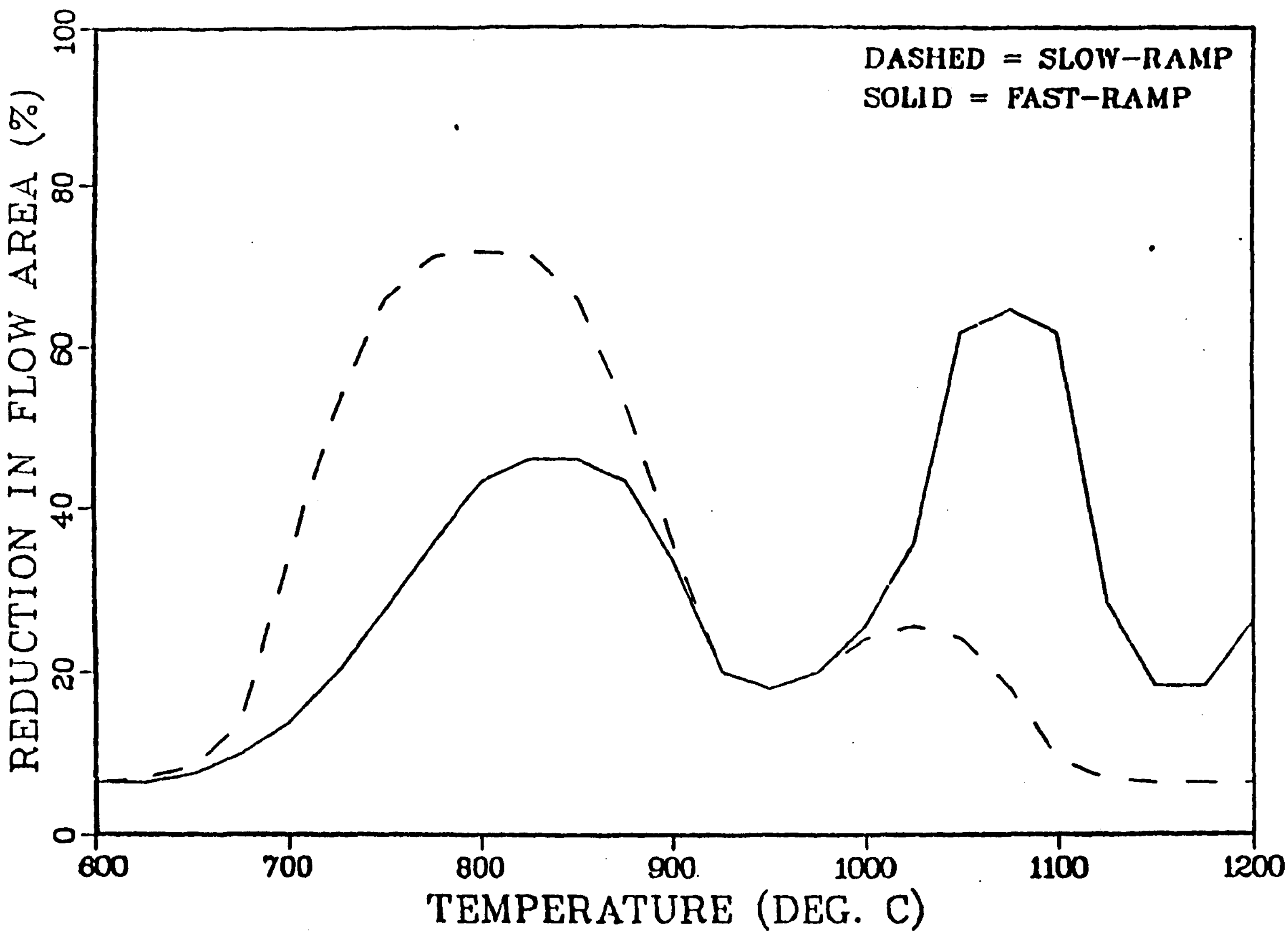

Fig. 4 Reduction in PWR assembly flow area as a function of rupture temperature and ramp rate.

metal-water reaction model is active; and additional form loss coefficients are (optionally) computed for the junctions just below and just above the rupture location,

K_e = $(1-B)^2$, expansion loss coefficient

K_c = $0.45(1-B)$, contraction loss coefficient

B = (Flow area after blockage/(Flow area before blockage)

The cladding deformation model does not alter any other parameters affecting the RELAP5 hydraulic solution. In particular it does not alter the flow area of the fluid cell containing a ruptured heat structure. Also, the geometric changes in a heat structure experiencing plastic deformation are not coupled to the geometry seen by the heat structures heat conduction solution. The geometry changes enter the conduction solution only by affecting the value being calculated for gap conductance.

When the reflood fine mesh rezoning algorithm is active the deformation model sees only the coarse zones. Deformation calculations are not done for each of the fine mesh points in a axial set of heat structures. Rather, the deformation calculation is done once for each of the axial heat structures and all of the fine mesh nodes within a particular heat structure have the same gap conductance value.

4. IMPLEMENTATION OF THE METAL WATER REACTION MODEL

Metal-water reaction rates are computed in subroutine QMWR. This subroutine is called once each time step for each heat structure requesting the metal-water reaction calculation. Subroutine QMWR has four calling parameters: Input parameters HINDEX (heat structure index) and DTIME (time step size); and output parameters QDI and QDO (the metal water reaction heat source for the cladding surface mesh point and outer surface mesh point, respectively).

Subroutine QMWR also loads several variables (Table 2) into the heat structure dynamic file. Thus the heat structure dynamic file was extended during implementation of the metal-water reaction model.

Subroutines HT1TDP and HT2TDP each cell QMWR to obtain the metal-water reaction's heat source for the cladding surfaces heat transfer nodes. The metal-water reaction heat source terms (QDI and QDO) returned by QMWR are added into the total nodal heat source term calculated by HT1TDP or HT2TAP.

The metal-water reaction model is activated for any slab by introducing a single card into the input for the heat slab (Table 3). This card is read and processed in subroutine HT1NIP. In particular, the initial oxide thickness for the outside surface of the heat structure is stored in the variables OXTO and OXTOO and the metal-water reaction flag bit in variable IWM is turned on.

Quantities calculated by subroutine QWMR are edited each major edit. The oxide thickness on the cladding's inner surface and the outer surface are given along with the total amount of hydrogen generated by all surfaces undergoing metal-water reaction.

The metal-water reaction model calculates the oxide thickness on the claddings' surfaces; however, it does not not alter the thermal-physical properties of the cladding as the oxide layers develop. Similarly, although the model calculates the amount of hydrogen freed from each

TABLE 2. VARIABLES ADDED TO THE HEAT STRUCTURE DYNAMIC FILE FOR THE METAL-WATER REACTION MODEL

Variable	Description
OXTI	New oxide thickness on the inner cladding surface
OXTO	New oxide thickness on the outer cladding surface
H2GEN	New value of total hydrogen generated by a slab
OXTIO	Old oxide thickness on the inner cladding surface
OXTOO	Repeat above statement outer
H2GENO	Old value of total hydrogen generated by a slab
IMW	Packed word containing metal-water reaction model flags and cladding deformation model flags.
	right 9 bits = mesh point number of inner cladding
	512 bit = on if rupture has occurred
	1024 bit = on if loss coefficients have changed
	2048 bit = on if plastic strain calculation requested
	4096 bit = on if loss coef to be altered after rupture
	8192 bit = on if mwr being calculated on inner surface
	16384 bit = on if mwr calculation requested.

TABLE 3. INPUT FOR THE METAL-WATER REACTION MODEL

Card 1CCCG003

Metal-water reaction control card. CCCG is a heat structure-geometry number. If this card is not present, no metal-water reaction will be calculated.

W1(R) OXTO

The initial oxide thickness on the cladding's outer surface.

surface undergoing metal-water reaction, this hydrogen does not get included into the RELAP5 hydraulic equations. Nor does the steam being consumed by the metal-water reaction get withdrawn from the hydraulic equations.

The metal-water reaction assumes there is always sufficient steam to allow the reaction to proceed. The model does not recognize the possibility of a reduced reaction rate due to insufficient available steam. The model does, however, recognize that the reaction is limited by the amount of cladding available. When all the cladding for a heat structure has been consumed the model terminates the metal-water reaction for that heat structure.

Table 4 shows the subroutines modified or added in order to implement the metal-water reaction model.

TABLE 4. SUBROUTINE INVOLVED IN THE METAL-WATER REACTION MODEL

HT1TDP	If advancement is successful then move save new values of oxide thicknesses and hydrogen generated. Call QMWR to get QDI and QDO (metal-water reaction heat source terms. Include QDI and QDO in nodal heat source terms of the conduction equation.
HT2TDP	Reflood heat transfer subroutine. Modified in a manner similar to HT1TAP.
HT1INP	Read and process the metal-water reaction control card.
RHTCMP	Initialize heat structure dynamic file variables.
MAJOUT	Include metal-water reaction edit.
QMWR	Calculates Oxide layer thickness, hydrogen generated and heat generated by metal-water reaction.

5. IMPLEMENTATION OF THE CLADDING DEFORMATION MODEL

In order to implement the cladding deformation model a number of subroutines were added to RELAP5, several existing subroutines were altered, and the heat structure dynamic file was expanded.

The principal outputs of the deformation model are stored in the heat structure dynamic file. Five words (Table 5) were added to the heat structure dynamic file during implementation of the deformation model.

The deformation model is activated for a heat structure via an additional input card (Table 6). This card is read and processed in subroutine HT1NIP. If the card is present and has one word on it then the appropriate bits in variable IMW are set to indicate the deformation model is to be used. The deformation model can be active for a heat structure only if the dynamic gap conductance calculation is requested for that heat structure.

The subroutines involved in the deformation model implementation are given in Table 7. This table shows how the subroutines are related to one another.

Subroutine HT1TDP assigns the cladding's heating rate, HETRAT, to the local variable DTDT, and calculates the average temperature of the cladding, CLTAVE. Subroutine HT1TDP passes the variables DTDT and CLTAVE to subroutine MADATA via the argument list. The flow area blockage, BLOCK, is returned from MADATA. If BLOCK is zero no further action is taken. If however, BLOCK is nonzero, then rupture has occurred and subroutine HT1TDP writes a message to that effect. It then calls subroutine KLOSS if a user has requested alteration of the local junctions' form loss factors. At the end of HT1TDP, after new nodal temperatures have been found, the cladding heating rate is determined and saved in the heat structure dynamic file (variable HETRAT). The heating rate is calculated by taking the average cladding temperature for the present time step, subtracting the previous time step's average cladding temperature and dividing the result by the time step size.

TABLE 5. VARIABLES ADDED TO THE HEAT STRUCTURE DYNAMIC FILE FOR THE CLADDING DEFORMATION MODEL

Variable	Description
GAPWD	Current width of the gap
CLADEX	Current deformed outer radius of the cladding (negative if rupture has occurred)
HETRAT	Cladding heating rate
STRNPL	Maximum plastic strain
IMW	Packed work containing metal-water reaction model flags and cladding deformation model flags
	right 9 bits = mesh point number of inner cladding
512 bit	= on if rupture has occurred
1024 bit	- on if loss coefficients have changed
2048 bit	= on if plastic strain calculation requested
4096 bit	= on if loss coefficient to be altered after rupture
8192 bit	= on if mwr being calculated on inner surface
16384 bit	= if mwr calculation requested

TABLE 6. INPUT FOR THE CLADDING DEFORMATION MODEL

Card 1CCCG004

Deformation model control card. CCCG is a heat structure-geometry number. If this card is not present, no deformation calculations will be done. If this card is present then card 1CCCG001 must also be present.

W1(I) KFLAG

Enter 0 if no additional form loss factors are to be calculated after a rod ruptures. Enter 1 if additional form loss factors are to be calculated. Either a 0 or a 1 must be entered.

TABLE 7. SUBROUTINES INVOLVED IN THE DEFORMATION MODEL

HT1TDP	Calculate CLTAVE and DTDT. Call MADATA for material properties. Set flags in IMW. Save heating rate in HETRAT. Call KLOSS for additional form loss factors if rupture has occurred and user requested calculation. Write message when rupture occurs.
MADATA	Call GAPCON and pass CLTAVE and DTDT to GAPCON.
GAPCON	Calculate gap conductivity. Call CPLEXP to get plastic strain and flow blockage. Store maximum plastic strain in STRNPL, gap width in GAPWD and cladding outer radius (deformed radius) in CLADEX.
CPLEXP	Set plastic strain and flow blockage induced during the current time step. Call RUPLAS to get the rupture temperature and temperature at which plastic strain begins. Call PLSTRN to get plastic strain and flow blockage.
RUPLAS	Calculates rupture temperature and temperature at which plastic deformation begins.
PLSTRN	Performs interpolations to determine the plastic strain and, if rupture has occurred, the flow blockage.
HT2TDP	Reflood heat transfer subroutine. Saves the current cladding heating rate in HETRAT.
MDATA2	Called by HT2TDP for material properties. If the deformation model is active then call calculate CLTAVE and DTDT and call GAPCON to calculate the gap conductance. Call GAPCON only once for each heat structure and assign a single gap conductance value to all fine mesh points with the structure.
HT1INP	Read and process the cladding deformation control card.
RHTCMP	Initialize heat structure dynamic file variables.
MAJOUT	Print the gap deformation model edit.

MADATA calls subroutine GAPCON to obtain the gap conductance. The only modification to MADATA was to define local variables TFUEL and TCLAD to be the fuel surface and cladding inner surface temperatures, respectively, and to change the argument list for the call to GAPCON so that the variables TFUEL, TCLAD, DTDT, and CLTAVE could be passed to GAPCON along with the plastic strain and rupture flags IPLAS and IRUPT.

Because of differences in the logic of the reflood heat transfer and the normal heat transfer in RELAP5 the deformation model had to be implemented somewhat differently in the two packages. In the reflood package the subroutine HT2TDP was changed only slightly so that the cladding heating rate (HETRAT) could be saved. MDATA2, on the other hand, was changed extensively.

MDATA2 is the subroutine in the RELAP5 reflood package which calculates material properties for heat structures. This subroutine was altered by appending a block of coding which is executed only if the deformation model is active. This block of coding consists of looping over all the axial nodes in a reflood set. If an axial node belongs to the same heat structure as a previous axial node then the gap conductance for the previous zone is assigned as this zone's gap conductance. On the other hand if an axial node does not belong to the same heat structure as a previous axial node then MDATA2 assigns the cladding heatup rate to local variable DTDT and computes the average cladding temperature for the axial midpoint of the heat structure. Next, GAPCON is called to find the gap conductance at the axial midpoint of the structure and to determine if cladding rupture has occurred. The gap conductance returned by GAPCON is assigned to the axial node. If rupture has occurred then a message to that effect is printed and subroutine KLOSS is called if a user has requested alternation of the local junctions form loss factors.

It is important to note that the procedure in MDATA2 assigns a common gap conductance to each fine mesh node belonging to a common axial heat structure. The deformation model considers only the heat structure average node and not individual axial nodes within the structure.

For both the normal and reflood heat transfer packages it is subroutine GAPCON which computes gap conductance and gap dimensions. This subroutine has been altered to include radiation across the gap into the gap conductance calculation and, if the deformation model is active, to include the deformation of the cladding into the gap conductance calculation.

GAPCON calls subroutine CPLEXP if the cladding deformation model is active. The average cladding temperature, CLTAVE, the cladding heating rate, DTDT, and the local hoop stress, TERM1, are passed to subroutine CPLEXP via the argument list.

CPLEXP sets the plastic strain and the flow blockage to zero if the cladding's hoop stress is not positive. If the hoop stress is positive then CPLEXP calls subroutine RUPLAS to obtain the temperatures at which rupture occurs, TRUPK, and the temperature at which plastic strain begins, TPLASK. These two temperatures are dependent on the heating rate and the hoop strain and are determined according to the equations given in Section pp.

After subroutine RUPLAS returns the values of TRUPK and TPLASK subroutine CPLEXP passes these values to subroutine PLSTRN along with the heating rate, DTDT, and the cladding temperature, CLTAVE.

Subroutine PLSTRN determines if the cladding is undergoing plastic deformation and whether or not the cladding has ruptured.

It returns the plastic strain, EPLAS, as a nonzero quantity if the cladding is experiencing plastic strain. If the cladding has ruptured then a nonzero flow area blockage, BLOCK is returned. Subroutine CPLEXP returns to subroutine GAPCON immediately after having set the values of EPLAS and BLOCK.

Once subroutine GAPCON has a value for EPLAS from subroutine CPLEXP it compares the value to the maximum plastic strain (STRNPL) thus far experienced by the cladding. If the current plastic strain is greater than the maximum the current value is assigned to STRNPL. If the current value is less than the previous maximum then the current value is changed to be the maximum previous strain. Next, the new radius of the cladding and the new width of the gap are calculated. The calculational procedure ensures than the gap width does not diminish once plastic deformation begins. The outer (deformed) clad radius for a heat structure is stored in variable CLADEX and the gap width is stored in variable GAPWD.

If PLSTRN returns to subroutine GAPCON with a nonzero value for BLOCK then a flag is set to show that the heat structure is ruptured. Subsequent calls to GAPCON for this heat structure will bypass the plastic strain calculations and thermal and elastic strain calculations; gap conductance will consider only the deformed cladding radius insofar as geometry calculations are concerned.

6. DEVELOPMENTAL ASSESSMENT

Developmental assessment was conducted to ensure that the metal-water reaction model and the cladding deformation model performed correctly.

6.1 Metal-Water Reaction Model Assessment

The assessment case (Table 8) for testing the metal-water reaction coding consisted of a single zircaloy-clad unpowered fuel rod imbedded in an constant temperature steam atmosphere. The heat capacity of the zircaloy was input as a very large number so that the cladding would remain at a constant temperature as the metal-water reaction proceeded.

Figure 5 compares the oxide thickness calculated by RELAP5 with measured values obtained from Reference 2. The good agreement between the measured and calculated values demonstrates that the Cathcart-Pawel correlation has been implemented correctly.

In order to demonstrate the metal-water reaction model was properly coupled to the heat conduction solution the test problem was run for a single time step (0.0 to 0.1 s) and the heat rise in the cladding was compared to a hand calculation. For this case the heat capacity of the cladding was restored to its actual value (35 BTU/lb/F). The thermal conductivity of the cladding was multiplied by 10^{-6} so that all the heat deposited in the outer cladding node would have to remain in that node. Thus, only the outer node of the cladding needed to be considered in the hand calculation of temperature rise. At 0.1 s RELAP5 calculated the outer cladding node to be 1712.2 K, an increase in 135.2 K from its initial value. The temperature rise, ΔT, calculated by hand from

$$\alpha * C_p * V_i * \Delta T = S_{mwr} - S_{out}$$

where

α = zircaloy density, 6500 kg/m^3

Table 8 RELAP5 Input for Testing the Metal-Water Reaction Model

```
= relap5          -   rod at fixed temp 1304 C
*****************************************************************
100      new transnt
101      run
102      british si
120      1010000  0.0  water  oncethru
201      160.  1.e-7  .10  00003  100   100  1000
*****************************************************************
*  minor edits  **************************************************
*****************************************************************
328      httemp   002100110
*****************************************************************
*  trip cards  ***************************************************
*****************************************************************
501      time           0  gt  null  0  300.   1
510      time           0  gt  null  0  0.   1
600      501
*****************************************************************
*  index of hydronamic components  *******************************
*****************************************************************
0010000  corout  tmdpvol
0030000  upplen  branch
0040000  core    pipe
0050000  loplen  branch
0060000  driver  tmdpjun
0070000  corein  tmdpvol
*****************************************************************
*  upper plenum sink  ***************  tmdpvol  *****************
*****************************************************************
0010101  0.  4.  2.78  0.  90.  4.  1.5e-4  0.  00
0010200  3
0010201  0.  600.  2379.
*****************************************************************
*  upper plenum  *******************  branch  ********************
*****************************************************************
0030001  2  1
0030101  0.   4.  2.78  0.  90.  4.   1.5e-4  0.  00
0030200  3  600.  2379.
0031101  003010000  001000000 .6950  0.0  0.0  31000
0032101  004010000  003000000 .0789  8.8  0.5  31000
0031201  0.0  .8324  0.
0032201  0.0  .8324  0.
*****************************************************************
*  core channel  ******************  pipe  ***********************
*****************************************************************
0040001  1
0040101  .109889  1
0040301  12.5     1
0040601  90.      1
0040801  1.5e-4  .24984  1
0041001  00  1
0041201  3  600.  2379.  0.0  0.0  0.0  1
*****************************************************************
*  lower plenum  ***********************  branch  ****************
*****************************************************************
0050001  1  0
0050101  .21  4.  0.  0.  90.  4.  1.5e-4  0.  00
0050200  3  600.  2379.
0051101  005010000  004000000  .04125  1.4  1.9  31100
0051201   6.   6.  0.
*****************************************************************
*  driver  *********************  tmdpjun  **********************
*****************************************************************
0060101  007000000  005000000  .04125
0060200  0.
0060201  0.  16.  16.  0.
*****************************************************************
*  lower plenum sink  **************  tmdpvol  ******************
*****************************************************************
0070101  .21  4.  0.  0.  90.  4.  1.5e-4  0  00
0070200  3
0070201  0.  600.  2379.
*****************************************************************
*****************************************************************
*  low power rods  *****************  heat structure  ***********
*****************************************************************
10021000  1  10  2  0  0. * 510  1   8
10021001  1200. 4010000
10021011  0. 0. 0. 0. 1
10021003  .0
10021100  0  1
10021101  6 .017083  1 .017458  2 .020125
10021201   1 6 2 7   3 9
10021301  .166667 6  0. 9
10021401  2379. 10
10021501  000000000  00000  0  1  12.5   1
10021601  004010000  10000  1  0  12.5  1
10021701  1  .0  0.  0.  1
10021901  0  .0446155  .0543147   0.0  1
*****************************************************************
*  material properties tables  ******  table  *******************
*****************************************************************
20100100  uo2
20100200  tbl/fctn  3   1        * gas mixture
20100201  nitrogen  0.4
20100202  xenon     0.6
20100251  7.5000e-5
20100300  tbl/fctn  1  1
20100301  0.005       *thermal conductivity
20100351  35.e6      *rho*cp*e6
*****************************************************************
*  power table  ********************  general table  ************
*****************************************************************
20200100  power
20200101  .0  1.8
.
```

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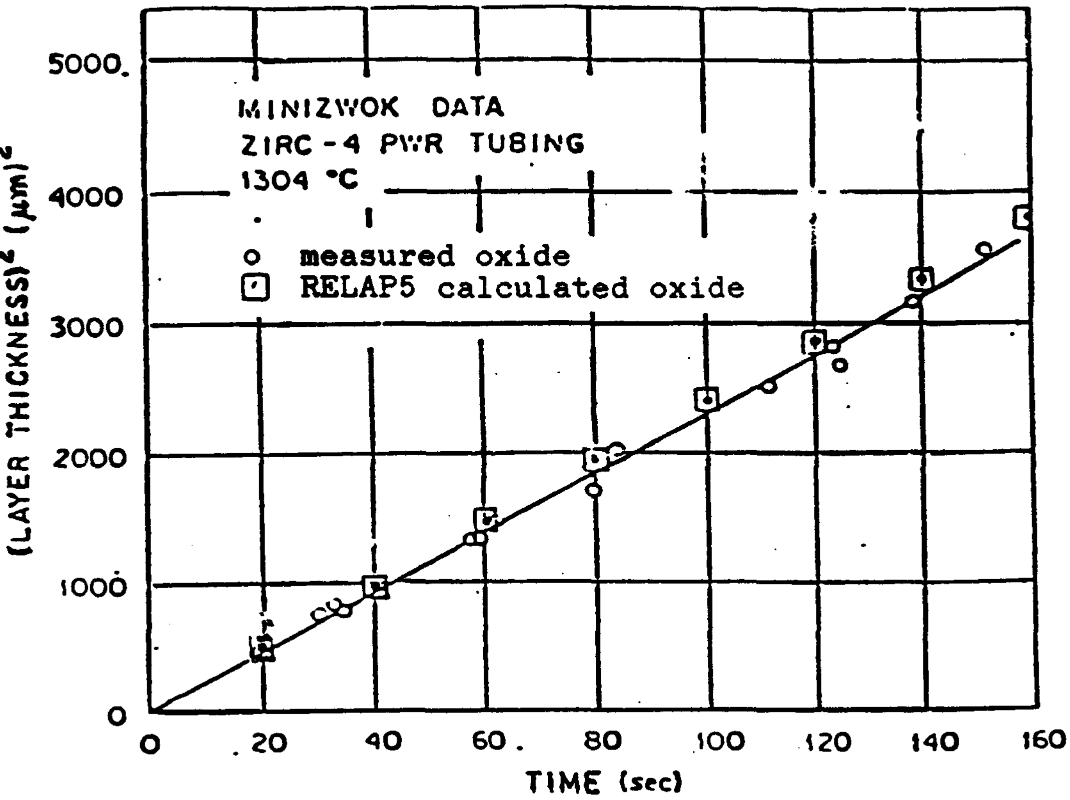

time(s)	thickness(μm)^2
20	478
40	956
60	1434
80	1913
100	2391
120	2869
140	3347
160	3825

Figure 5. Comparison of Calculated and Measured Oxide Layer (Original Plot Reproduced form Reference 2)

C_p = zircaloy heat capacity, 361.1 J/kg/K

V_i = volume of outer node, 7.70E-6 m^3/m

S_{mwr} = heat from metal-water reaction, 2522.4 J/m

S_{out} = heat loss to fluid, 0.0 J/m.

gave a temperature rise of 139.4 K and a temperature of 1716.4 K at 0.1 s. The good agreement of this value with the RELAP5 value demonstrated that the metal-water reaction model was properly coupled with the heat conduction solution. The RELAP5 case was run twice, with and without the reflood package activated. Thus, it was demonstrated that metal-water reaction model was coupled properly with both the one-dimensional heat conduction solution and the two-dimensional (reflood) heat conduction solution.

6.2 Cladding Deformation Model Assessment

The input for the cladding deformation test case is given in Table 9. The test case consists of two powered rods imbedded in an isobaric (4.1 MPa) steam atmosphere. The rods are initially pressurized to 8.3 Mpa (low power rods) or 13.8 MPa (high power rods). The test problem was run to 40 s, long enough to obtain rupture in both sets of rods.

The calculated behavior of the high powered rod is shown in Figure 6. This rod ruptured at axial Level 5 and 17.9 s. When rupture occurred the cladding temperature rise at Level 5 was terminated because the cladding ballooned and the gap between the fuel and the cladding increased. The temperatures at Levels 6 and 7 increased sharply when the rod ruptured. This occurred because the elastic strain on the cladding disappeared when the rod ruptured and the gap width diminished at Levels 6 and 7. For the high powered, highly pressurized rod plastic deformation of the cladding was limited to axial Level 5.

Table 9 RELAP5 Input for Testing the Cladding Deformation Model.

```
= relap5 clad swelling, reflood and rupture sample problem
*  gapinp
************************************************************
100      new transnt
101      run
102      british si
120      1010000  0.0  water  oncethru
201      31.  1.e-7  .10  00003  1   50  100
************************************************************
*  minor edits  ********************************************
************************************************************
328      httemp   002100110
329      httemp   002100210
330      httemp   002100310
331      httemp   002100410
332      httemp   002100510
333      httemp   002100610
334      httemp   002100710
335      httemp   002100810
337      httemp   003100110
338      httemp   003100210
339      httemp   003100310
340      httemp   003100410
341      httemp   003100510
342      httemp   003100610
343      httemp   003100710
344      httemp   003100810
************************************************************
*  trip cards  *********************************************
************************************************************
501      time            0  gt  null  0  300.   1
510      time            0  gt  null  0  0.   1
502      httemp  3100810  gt  null  0  2000.  1
600      501 502
************************************************************
*  index of hydronamic components  *************************
************************************************************
0010000  corout  tmdpvol
0030000  upplen  branch
0040000  core    pipe
0050000  loplen  branch
0060000  driver  tmdpjun
0070000  corein  tmdpvol
************************************************************
*  upper plenum sink  ***************  tmdpvol  ************
************************************************************
0010101  0.  4.  2.78  0.  90.  4.  1.5e-4  0.  00
0010200  3
0010201  0.  600.  500.
************************************************************
*  upper plenum  *********************  branch  ************
************************************************************
0030001  2  1
0030101  0.   4.  2.78  0.  90.  4.   1.5e-4  0.  00
0030200  3  600.  500.
0031101  003010000  001000000 .6950  0.0  0.0  31000
0032101  004010000  003000000 .0789  0.3  0.5  31000
0031201  0.0  .8324  0.
0032201  0.0  .8324  0.
************************************************************
*  core channel  *********************  pipe  **************
************************************************************
0040001  8
0040101  .109889  8
0040301  1.5625   8
0040601  90.      8
0040801  1.5e-4  .24984  8
0040901  1.24  1.24  7
0041001  00  8
0041101  31000  7
0041201  3  600.  500.  0.0  0.0  0.0  8
0041300  1
0041301  0.0  .8324  0.  7
************************************************************
*  lower plenum  ************************  branch  *********
************************************************************
0050001  1  0
0050101  .21  4.  0.  0.  90.  4.  1.5e-4  0.  00
0050200  3  600.  500.
0051101  005010000  004000000  .04125  1.4  1.9  31100
0051201   6.   6.  0.
************************************************************
*  driver  **************************  tmdpjun  ************
************************************************************
0060101  007000000  005000000  .04125
0060200  0.
0060201  0.  16.  16.  0.
************************************************************
*  lower plenum sink  ***************  tmdpvol  ************
************************************************************
0070101  .21  4.  0.  0.  90.  4.  1.5e-4  0  00
0070200  3
0070201  0.  600.  500.
************************************************************
*  channel walls  ********************  heat structure  ****
************************************************************
10011000  8  3  2  0  0.
10011100  0  1
10011101  2  .0066667
10011201  3  2
10011301  0. 2
10011401  500.  3
10011501  000000000  00000  0  1  1.5625  8
10011601  004010000  10000  1  0  2.74896  8
10011701  0  0.  0.  0.  8
10011901  0  .24984  0  0.0  8
```

Table 9 (continued)

```
*******************************************************************************
*  low power rods  *******************  heat structure  *******************
*******************************************************************************
10021000  8  10  2  0  0.  510  1  8
10021001  1200.  4080000          * internal rod pressure
10021003  .0
10021004  1
10021011  0.0  0.0  0.0  0.0   8
10021100  0  1
10021101  6 .017083  1 .017458  2 .020125
10021201  1 6  2 7  3 9
10021301  .166667 6  0. 9
10021401  501. 10
10021501  000000000  00000  0  1  1.5625   8
10021601  004010000  10000  1  0  10.6692  8
10021701  1  .054486  0.  0.  1
10021702  1  .098586  0.  0.  2
10021703  1  .131186  0.  0.  3
10021704  1  .148514  0.  0.  4
10021705  1  .148514  0.  0.  5
10021706  1  .131186  0.  0.  6
10021707  1  .098586  0.  0.  7
10021708  1  .054486  0.  0.  8
10021901  0  .0446155  .0543147   0.0  8
*******************************************************************************
*  high power rods  *******************  heat structure  ******************
*******************************************************************************
10031000  8  10  2  0  0.  510  1  8
10031001  2000.  4080000
10031003  .0
10031004  1
10031011  0.0  0.0  0.0  0.0  8
10031100  0  1
10031101  6 .017083  1 .017458  2 .020125
10031201  1 6  2 7  3 9
10031301  .166667 6  0. 9
10031401  501. 10
10031501  000000000  00000  0  1  1.5625  8
10031601  004010000  10000  1  0  1.58061 8
10031701  1  .008463  0.  0.  1
10031702  1  .015314  0.  0.  2
10031703  1  .020378  0.  0.  3
10031704  1  .023069  0.  0.  4
10031705  1  .023069  0.  0.  5
10031706  1  .020378  0.  0.  6
10031707  1  .015314  0.  0.  7
10031708  1  .008463  0.  0.  8
10031901  0  .0446155  .0543147   0.0  8
*******************************************************************************
*  material properties tables  ******  table  ****************************
*******************************************************************************
20100100  uo2
20100200  tbl/fctn  3  1        * gas mixture
20100201  nitrogen  0.4
20100202  xenon     0.6
20100251  7.5000e-5
20100300  zr
*******************************************************************************
*  power table  **********************  general table  *******************
*******************************************************************************
20200100  power
20200101  .0  1.8
.
```

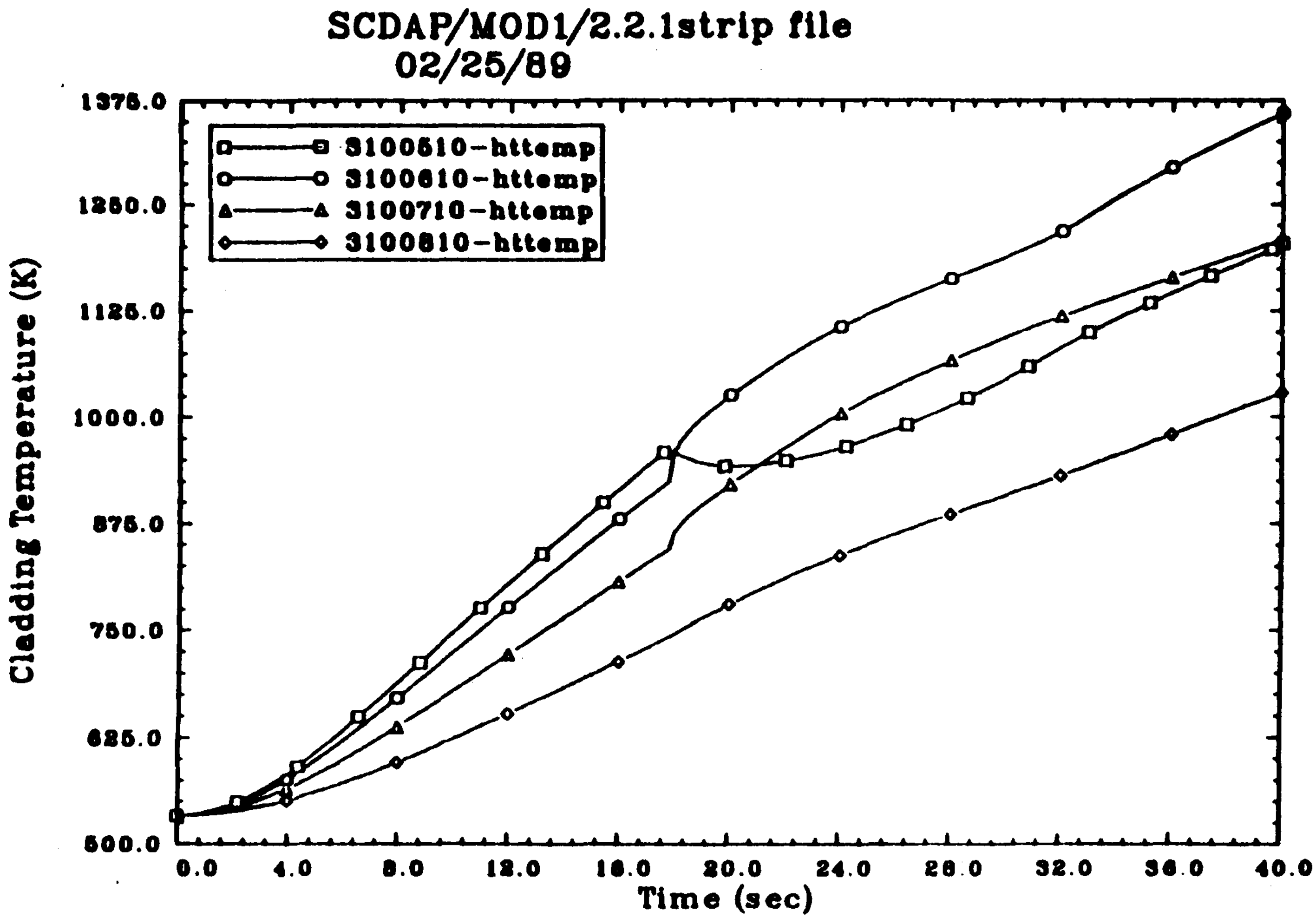

Figure 6 Calculated Cladding Temperature for the High Powered Rod.

The low powered rod behaved quite differently from the high powered rod - it underwent significant plastic deformation over much of its length before rupturing. The behavior calculated for the upper part of the low powered rod is illustrated in Figure 7. The onset of plastic deformation at axial Levels 5, 6, and 7 arrested the rapidly rising cladding temperatures at these levels. Once the deformation had stabilized and a new temperature distribution was established in the fuel the cladding temperatures began to rise again. Rupture occurred at axial Level 5 at 34.4 s. A slight rise in the Level 5 cladding temperature occurred at rupture because metal-water reaction was then activated on the inside surface of the cladding.

The effect which the deformation model can have on cladding temperature is shown in Figure 8. This figure shows the calculated temperatures at axial Level 5 of the low powered rod for four cases: A base case having no metal-water reaction or cladding deformation; a case with metal-water reaction only; a case with metal-water reaction and cladding deformation; and a case with metal-water reaction, cladding deformation and reflood. The good agreement between the latter two cases demonstrates that the deformation model has been implemented consistently into both the normal heat transfer package and the reflood heat transfer package.

A final check on the deformation model was conducted by comparing the updated version of RELAP5 with the unupdated version. In both of these cases the metal-water reaction models and the cladding deformation models were not active. These two cases produced identical results (Figure 9) demonstrating that the coding done to implement the models has no effect on computed results when the models are turned off.

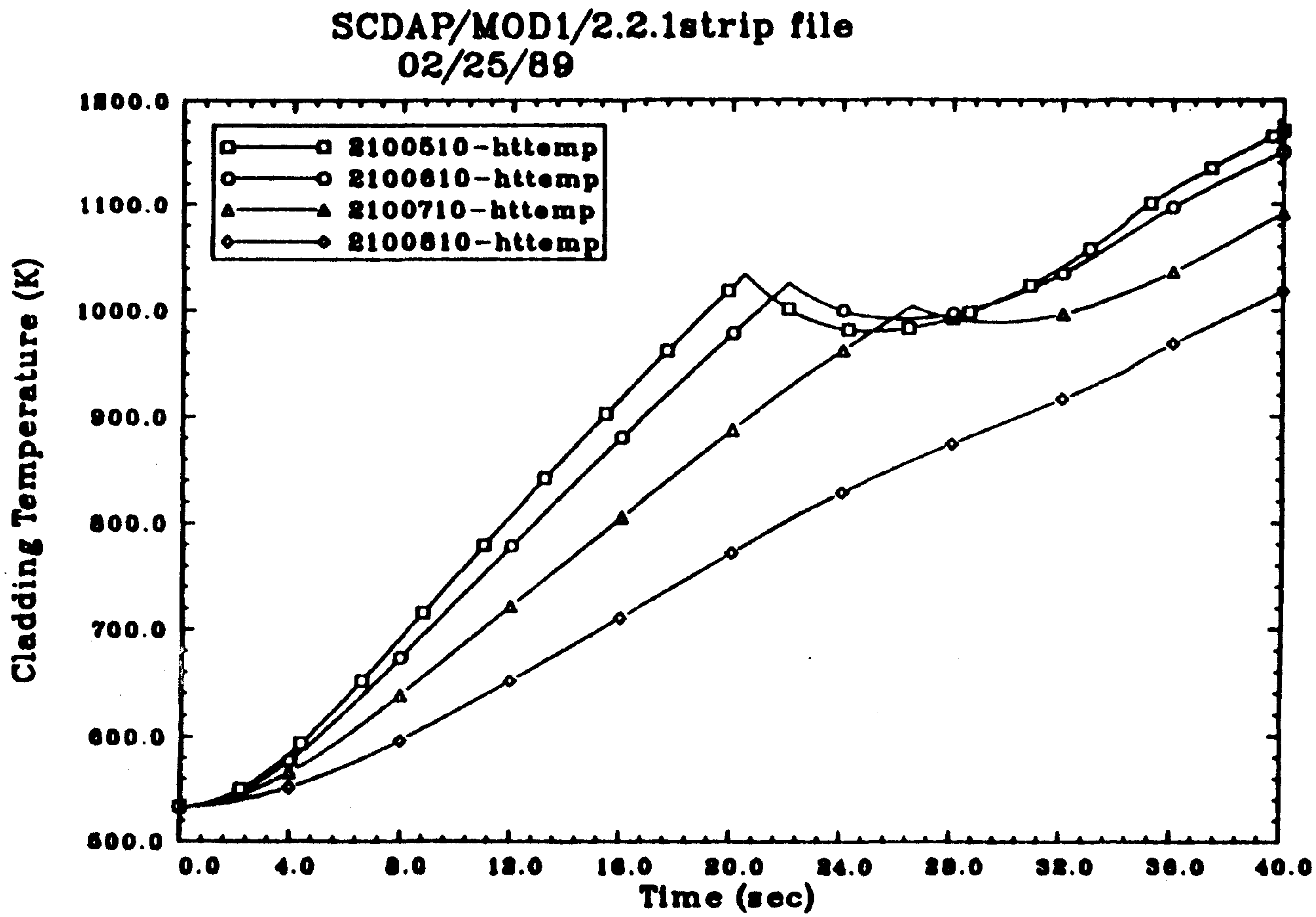

Figure 7 Calculated Cladding Temperature for the Low Powered Rod.

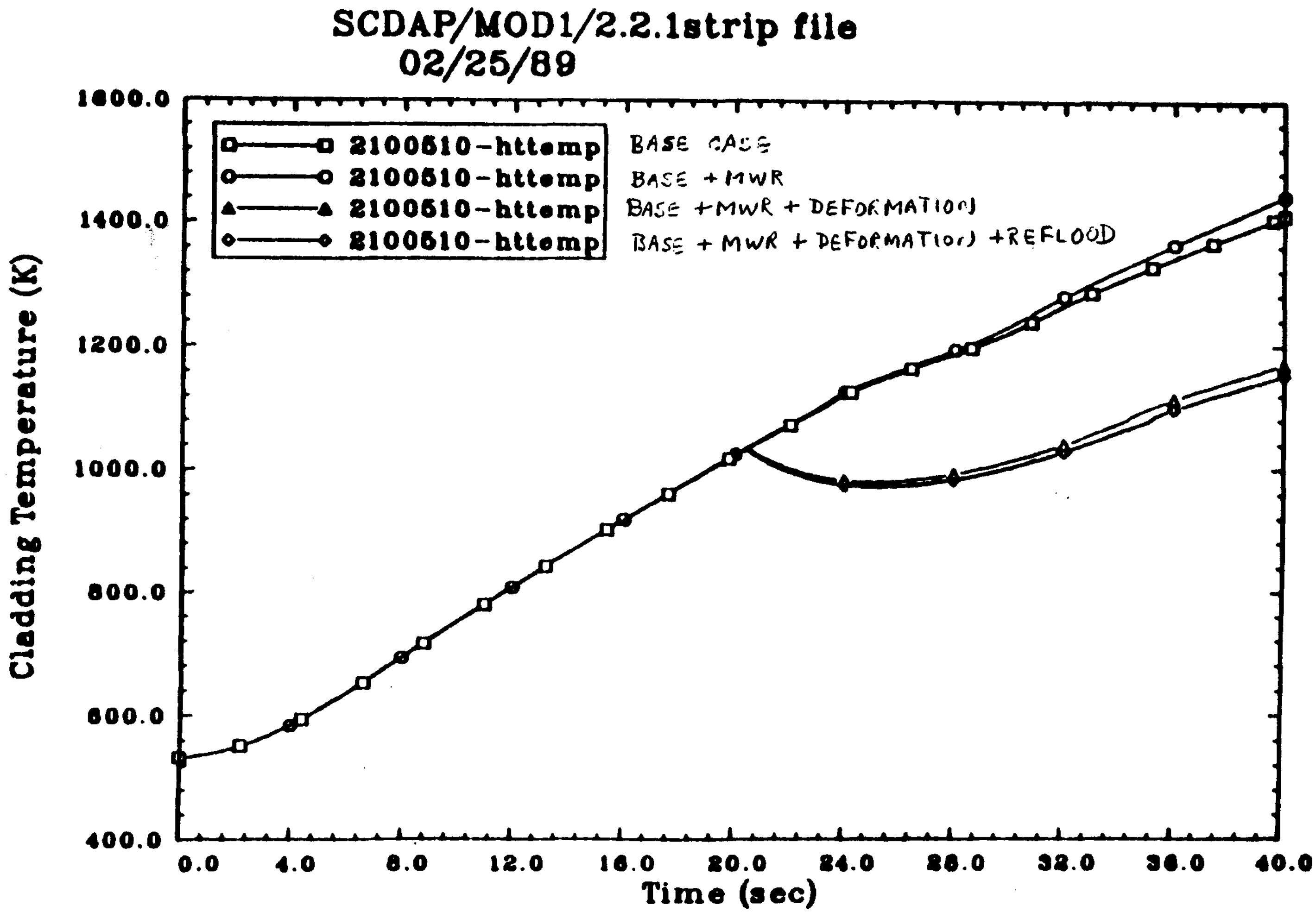

Figure 8 Calculated Cladding Temperature at Level 5 of the Low Powered Rod for the Four Cases.

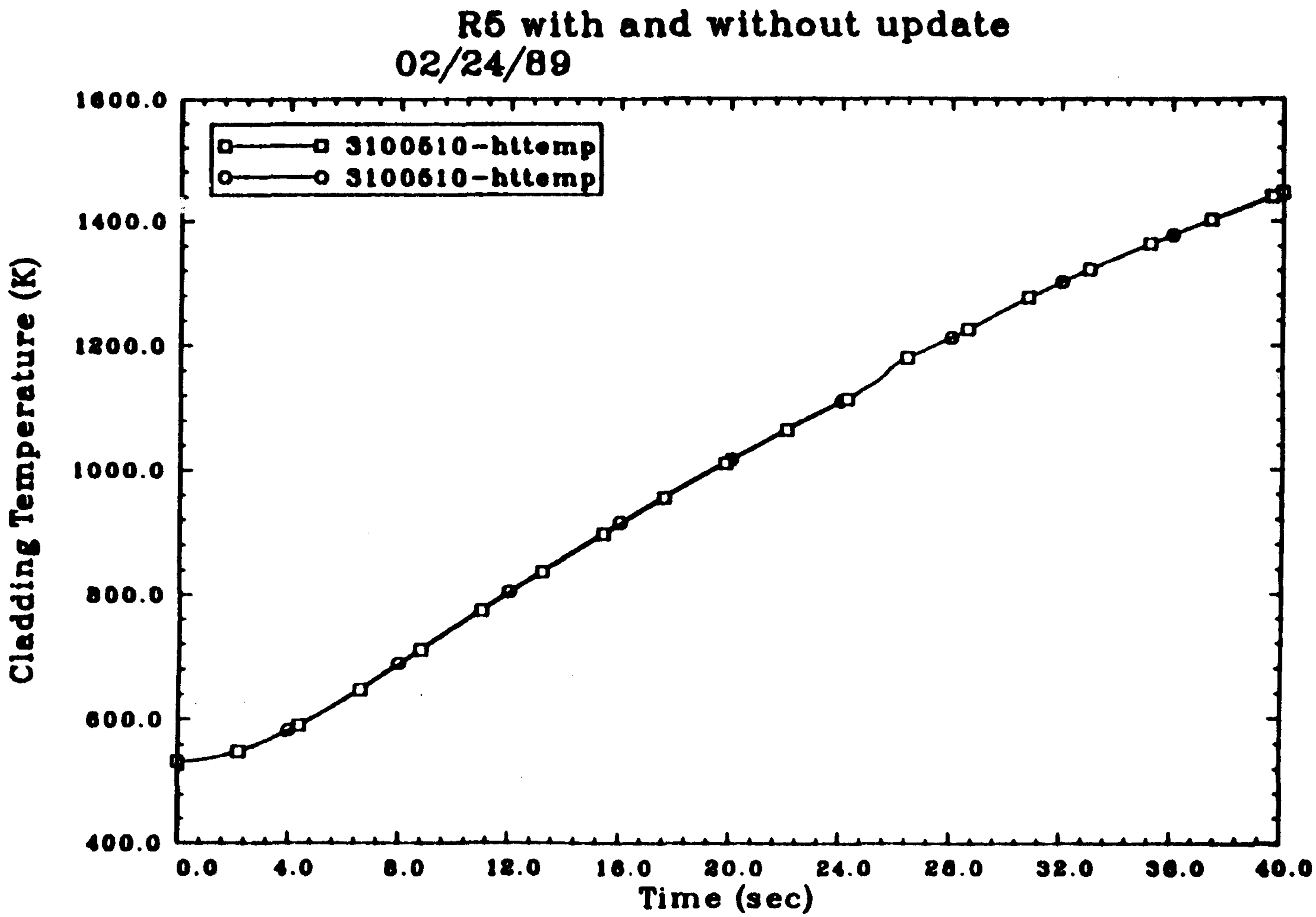

Figure 9 Calculated Cladding Temperatures with Two Versions of RELAP5.

7. REFERENCES

1. Ransom et. al., RELAP5/MOD2 Code Manual.

2. J. V. Cathcart et al., Reaction Rate Studies, IV, Zirconium Metal-Water Oxidation Kinetics, ORNL/NUREG-17, August 1977.

3. S. C. Resch et. al., FRAP-T6: The Transient Fuel Rod Behavior Code, NUREG/CR-2950, September 1982.

4. D. A. Powers and R. O. Meyer, Cladding Swelling and Rupture Models for LOCA Analysis, NUREG-0630, April 1980.