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### A THREE-DIMENSIONAL NODAL NEUTRON KINETICS CAPABILITY FOR RELAP51

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#### **ABSTRACT**

The incorporation of a three-dimensional neutron kinetics capability into the DOE version of the RELAP5/MOD3.2 reactor safety code is discussed. A brief discussion of the kinetics method is given along with a discussion of the cross section parameterization models available in RELAP5/MOD3.2. The RELAP5/MOD3.2 code is then used to perform calculations of the NEACRP rod ejection and rod withdrawal benchmarks, and results are presented.

#### INTRODUCTION

A three-dimensional nodal neutron kinetics module based on the NESTLE<sup>1</sup> computer code developed at North Carolina State University has been incorporated into the DOE version of RELAP5/MOD3.2<sup>2</sup> thermal hydraulics reactor safety code. This capability enables the analyst to perform best-estimate calculations for accidents such as Steam-Line Break, PWR Rod Ejection, and BWR Rod Drop, that have been performed in a conservative manner using point kinetics in the past.

#### NESTLE CAPABILITIES

The NESTLE code permits the analyst to model both cartesian and hexagonal geometries in three dimensions with reflective, cyclic, zero flux, and non-reetrant current boundary conditions. It allows quarter, half, and full core models in cartesian geometry and sixth, third, and full core models in hexagonal geometry. The code solves the diffusion equations in two or four energy groups, and all groups may be thermal with a full scatter matrix specified. The few-group neutron diffusion equations are spatially discretized utilizing the Nodal Expansion Method (NEM). Quartic or quadratic polynomial expansions for the transverse integrated fluxes are employed for cartesian or hexagonal geometries, respectively. Transverse leakage terms are represented by a quadratic polynomial for Cartesian geometry and are constant for hexagonal geometry. Assembly Discontinuity Factors (ADFs) are utilized to correct for homogenization errors. Time discretization is done in a fully implicit manner utilizing a first-order difference operator for the diffusion equation. The precursor equations are analytically solved assuming the fission rate behaves linearly over a time-step. Independent of problem type, an outer-inner iterative strategy is employed to solve the resulting matrix system. Outer iterations can employ Chebyshev acceleration to accelerate convergence. Inner iterations employ either color line or point SOR iteration schemes, dependent upon problem geometry. Values of the energy group dependent optimum relaxation parameter and the number of inner iterations per outer iteration to achieve a user specified L<sub>2</sub> error reduction are determined a priori. The non-linear iterative strategy associated with the NEM method is utilized. The user may elect not to update the coupling coefficients in the non-linear iterative strategy and solve the diffusion equations by the Finite Difference Method.

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#### KINETICS MODELING CAPABILITIES

A flexible macroscopic neutron cross section model has been developed which accepts neutron cross section data in three formats, a format developed at Brookhaven National Laboratory for BWR applications, a format at Argonne National Laboratory for analysis of the heavy water production reactors at Savannah River National Laboratory, and a third format developed especially for the RELAP5/MOD3 code at the Idaho National Engineering Laboratory. The BNL and ANL formats may be algebraically manipulated into the new INEL format, but the code accepts the BNL and ANL formats directly and performs the manipulation internally. The new format is also general enough to accommodate the cross section formulation contained in the NEACRP<sup>3</sup> benchmark problems. The INEL cross section model was used for the benchmarking and it is discussed in the following paragraphs.

The INEL cross section function formulation of the cross section is defined for three control states, active controlled, driver controlled and uncontrolled states. The INEL cross section function is given by

$$\Sigma_{l}^{x} = C_{fl}^{a} \Sigma_{xc}^{a} \left( 1 + \frac{\delta \Sigma_{xc}^{a}}{\Sigma_{xc}^{a}} \right) + \left( 1 - C_{fl}^{a} - C_{fl}^{d} \right) \Sigma_{xc}^{u} \left( 1 + \frac{\delta \Sigma_{xc}^{u}}{\Sigma_{xc}^{u}} \right) + C_{fl}^{d} \Sigma_{xn}^{d} \left( 1 + \frac{\delta \Sigma_{xc}^{d}}{\Sigma_{xc}^{d}} \right)$$
(1)

where,

C<sub>fl</sub><sup>a, d</sup> = control fraction for active and driver portions of the control rods in node l,

 $\Sigma_{xc}^{a, d, u}$  = base cross section of reaction type x for composition c for active controlled, driver controlled, or uncontrolled states, and

 $\delta \Sigma_{\rm xc}^{\rm a, d, u}$  = variation of cross section for reaction type x for composition c due the changes in the thermal-hydraulic variables from the base thermal-hydraulic state for active controlled, and uncontrolled states,

where composition c has been specified for node 1.

The variations for the active controlled, driver controlled, and uncontrolled states are given by Eqn () where the coefficients a,b,c,d, and e are input separately for the active controlled, driver controlled, and uncontrolled states. The density variable in the variation of the cross section may be either the fluid mixture density or the fluid void fraction and the variation of the structure temperature may be the difference of the structure temperature and the reference temperature or the difference of the square roots of the structure temperature and the reference temperature. The nodal discontinuity factors are also computed from Eqn () except that the thermal-hydraulic variations are identically zero and are therefore not included.

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$$\begin{split} \frac{\delta \Sigma_{xl}}{\Sigma_{xl}^{base}} &= \sum_{i \in N_v} a_{xin} \Delta T_{mik} + \sum_{i \in N_v} b_{xin} \Delta \bar{p}_{mik} + \sum_{i \in N_v} c_{xin} \left( \Delta \bar{p}_{mik} \right)^2 \\ &+ \sum_{i \in N_v} d_{xin} \Delta \bar{B}_{ik} + \sum_{i \in N_s} e_{xin} \sqrt{\Delta T_{sik}} \end{split} \tag{2}$$

where,

 $\Sigma_{x1}^{\text{base}}$  = base cross section of type x in node l,

 $\delta\Sigma_{x1}$  = change in cross section x in node l due to changes in the thermal-hydraulic state of the zone to which node l corresponds,

a<sub>xin</sub> = coefficient for change in cross section x of composition n due to change in average moderator temperature of region i,

 $\Delta T_{mik}$  = change in average moderator temperature in region i of zone k,

 $= T_{mik} - T_{min}^{base} ,$ 

 $T_{mik}$  = average moderator temperature in volume region i of zone k,

T<sup>base</sup> = average moderator temperature in volume region i for composition n at base thermal-hydraulic conditions, e.g. full power steady state,

 $N_v$  = number of volume regions in each zone,

b<sub>xin</sub> = linear coefficient in change of cross section x of composition n due to changes in average moderator density in volume region i,

 $\Delta \bar{p}_{mik}$  = change in average moderator density in volume region i of zone k,

 $= \bar{\rho}_{mik} - \bar{\rho}_{min}^{base}$ 

 $\bar{\rho}_{\min}^{\text{base}}$  = average moderator density in volume region i for composition n at base thermal-hydraulic state,

c<sub>xin</sub> = quadratic coefficient in change of cross section x of composition n due to changes in average moderator density in volume region i,

d<sub>xin</sub> = coefficient for change in cross section x of composition n due to changes in average poison density in volume region i,

 $\Delta B_{ik}$  = change in average poison concentration in volume region i of zone k,

	=	$B_{ik} - B_{in}^{base}$
B <sub>in</sub> <sup>base</sup>	<b>=</b>	average poison concentration in volume region i for composition n at base thermal-hydraulic condition,
e <sub>xin</sub>	=	coefficient for change in cross section x of composition n due to changes in average structure temperature of structure region i.
$\sqrt{\Delta T_{\rm sik}}$	=	change in the square root of the effective structure temperature in structure region i of zone k.
	=	$\sqrt{T_{sik}} - \sqrt{T_{sin}^{base}}$ ,
T <sub>sin</sub> <sup>base</sup>	= =	average structure temperature in structure region i of composition n for base thermal-hydraulic state, and
$N_s$	=	number of structure regions in each zone.

The nodalization is very flexible through the use of axial figures for the specification of compositions for each kinetics solution node in an axial plane as well as for the specification of which thermal-hydraulic variables to use for the calculation of neutron cross sections in each node. Compositions are defined as sets of coefficients in the cross section function while thermal hydraulic zones are defined as weighted averages of the thermal-hydraulic variables over a user input set of RELAP5 volumes and heat structures with user defined weighting factors. Each thermal-hydraulic zone may be comprised of several RELAP5 volumes and heat structures which may represent individual fluid subchannels and fuel rods, respectively if defined. There may be up to 9999 zones and 999 compositions in a problem with 999 axial levels. Each axial level may contain up to 9999 kinetics nodes.

The values of the neutron cross sections, neutron fluxes, nodal power, control rod positions, and thermal-hydraulic variables may be printed or plotted at the users direction through code input.

#### BENCHMARKING

The rod ejection and uncontrolled rod withdrawal accidents are standard Pressurized Water Reactor (PWR) safety analysis problems that require spatial kinetics because the core typically undergoes a significant power redistribution. A series of three PWR rod ejection transients from Hot Zero Power and Hot Full Power were proposed as a benchmark by the NEACRP3. We analyzed series A, the ejection of the central rod, and series B, the ejection of peripheral rods, using the spatial kinetics option of RELAP5. The location of the ejected control rods and the initial core configuration is shown in Figure 1 and a complete description of the problem is provided in Reference 3. For the series A and B transients one-quarter core geometry was adequate. Reference 4 specifies a series of rod withdrawal transients using the same cross sections and geometry as specified in Reference 3.

### RELAP5 THERMAL HYDRAULIC CORE MODELING

Our RELAP5 core model for the benchmark problem consisted of a sequence of parallel pipes as shown in Figure 2. Each pipe was constructed using a series of heat structures and control volumes to describe the fuel and coolant from a single fuel assembly. A separate inlet reservoir was provided for each pipe and was set at a constant pressure, temperature, and boron concentration. Each pipe was connected to

its reservoir using a time dependent junction which provided identical, constant flow to each assembly. The outlet of each pipe was connected to an outlet reservoir using a series of branches. Since a maximum of 9 junctions per branch are allowed, we used additional branches to accommodate the total of 47 pipes for our quarter core model.

During the course of our analysis, we examined various thermal-hydraulic mesh structures. The finest axial mesh used for the pipes corresponds to that prescribed in the NEACRP problem with the exception that the three smallest nodes at the bottom and top of the core were combined into a single thermal-hydraulic nodes. We retained the original NEACRP mesh structure for the neutronic solution. This provided for a total of 14 axial thermal-hydraulic mesh in each pipe. For purposes of the thermal-hydraulic calculation, the reflector was modeled as a separate, single pipe because we anticipated a very small temperature rise in the reflector.

For the fuel pin model we used 8, 1, and 2 mesh in the fuel pellet, gap, and cladding, respectively. In order to generate an effective Doppler temperature in RELAP5 consistent with that prescribed in the NEACRP problem,

$$T = (1 - \alpha) T_{F,C} + \alpha T_{F,S}$$

we used very small central and peripheral fuel pellet mesh such that the area of these regions corresponds to the weighting of the surface,  $T_{F,S}$ , and centerline fuel temperature,  $T_{F,C}$  specified in the benchmark problem. All other fuel pellet mesh were equidistant.

Because the benchmark problem specifies gap conductance and RELAP5 only accepts gap conductivity, the following relation was used:

$$k = h\Delta r$$

where k and h are the gap conductivity and conductance, respectively, and  $\Delta r$  is the gap width. This expression is valid for a small gap width as used in the benchmark problem.

#### **NEUTRONIC MODELING**

The neutron flux solution was obtained using the Nodal Expansion Method (NEM) and the non-linear iterative technique discussed earlier. The coupling coefficients are periodically updated during the outer iterations

The axial mesh structure used for the neutronic solution was identical to that specified in the benchmark problem and four nodes per fuel assembly were used in the radial plane. The partial cross sections prescribed in the NEACRP benchmark were processed into an equivalent set of cross section multipliers to coincide with the modeling used in RELAP5. Some minor discrepancy persisted since it is not possible to construct a completely consistent set of partial cross section data for the diffusion coefficient used in RELAP5 based on the partial transport cross section data specified in the benchmark problem.

#### ROD EJECTION RESULTS

The steady state solution was obtained by running a null transient with RELAP5 for 100 seconds using time steps of 0.05 secs. The current algorithm provides for a thermal-hydraulics update only at the completion of each k-effective solution. The convergence criteria for the neutronic solution was set at 10<sup>-4</sup> and 10<sup>-5</sup> for the global fission source and k-effective, respectively. The coupling coefficients in the NEM nonlinear iteration method were updated every five outer iterations. For the transient solution, the global fission source convergence criteria was increased to 10<sup>-5</sup>. The time step sizes for the transients are given in Table 1.

Table 1. Time Step Sizes Used in the Rod Ejection Analyses

Case	0 to 1 second	1 to 5 seconds
Zero Power (A1, B1)	0.001	0.01
Full Power (A2, B2)	0.01	0.05

The results of the four transients cases are summarized in Table 2. The reference results are those reported at the Karlsruhe conference5. The transient power for each of the four cases is compared with the reference in Figure 3 for A1 and A2 and in Figure 4 for B1 and B2. The RELAP5 radial power distribution at axial plane 6 (out of 16) for problem A1 is compared to the reference in Figure 5 for the steady state (t=0), for the maximum power condition (t=0.611 secs), and for the asymptotic core state (t=5 secs).

Table 2. Summary of the RELAP5 NEACRP Rod Ejection Benchmark Calculation Results

	A1		B1		A2		B2	
Steady State								
Critical Boron Conc. (ppm)	563.4	-4.6	1253	-1.4	1154	-6.8	1183	-4.8
Assembly Peaking Factor	2.865	0.3%	1.926	-0.2%	2.203	-0.8%	2.101	-0.4%
Max. Fuel. Temperature (C)	286.0	0.0%	286.0	0.0%	1612	-3.6%	1528	-3.1%
Rod Worth (pcm)	820	-0.2%	836	0.6%	91	1.7%	99	-0.1%
@ Time of Maximum Power								
Time (sec)	0.573	0.013	0.500	-0.02	0.095	-0.025	0.100	-0.020
Relative Core Power	1.082	-7.4%	2.574	5.3%	1.085	0.7%	1.065	0.2%
Max. Fuel Temperature (c)	337.2	-2.3%	325.5	-0.9%	1613	-3.5%	1528	-3.1%
@ Time = 5.0 sec								
Relative Core Power	0.188	-3.6%	0.312	-2.4%	1.036	0.0%	1.038	0.0%
Max. Fuel Temperature (C)	650.0	-3.2%	549.9	-1.5%	1632	-3.5%	1539	-3.1%

As indicated in Table 2, the RELAP5 steady state results for the hot zero power cases are in reasonably good agreement with the reference results. RELAP5 does show a slight negative bias in the prediction of the critical boron concentration for both cases A1 and B1. The RELAP5 ejected rod worth prediction for both cases is in good agreement with the reference result. RELAP5 predicts the maximum power will occur 0.013 seconds later and have a magnitude 7.4% lower than the reference calculation.

The asymptotic core state predicted by RELAP5 is in reasonably good agreement with the reference result as shown in Table 1, although RELAP5 shows a slight negative bias in the asymptotic core power.

The RELAP5 steady state results for the hot full power cases show a slight negative bias in the prediction of the critical boron concentration. As shown in Figure 4, the RELAP5 transient results for cases A2 and B2 are in close agreement with the reference results. As shown in Table 2, there is good agreement between RELAP5 and the reference in the prediction of the time of the maximum power, as well as in the prediction of the asymptotic core power.

#### ROD WITHDRAWAL RESULTS

The rod withdrawal model is identical to the rod ejection model with the exception that the control rod in the center fuel assembly is removed from the model. Four different benchmark problems were defined in the specification, but only three are shown in this paper. The fourth problem was just a variation in the core heat transfer coefficient that did not change the results of the transient. Initial rod bank positions and the banks withdrawn for the three analyzed cases are given in Table 3. The rods are withdrawn from the core at 72 steps/minute. The reactor trip is at 35% power. The rods begin to fall 0.6 seconds after the trip at a constant rate of 228 steps in 2.2 seconds.

	C	Banks to				
Case	D	С	В	A	S	Withdraw
A	228	0	0	0	0	A
В	228	228	228	228	. 0	B, C
D	228	228	228	228	0	A. B

Table 3. Initial Rod Bank Positions for the Rod Withdrawal Benchmark Problems.

Figure 5 shows the results for case A compared to the reference data. The RELAP5 calculation predicts the power increase approximately 3 seconds later than the reference, but the overall behavior is predicted quite well. Figure 6 presents the results for case B. Once again, the power increase in RELAP5 is approximately 3 seconds after the reference, but the peak power is significantly underpredicted. Figure 7 shows the results for case D. The peak power for this case is overpredicted and the power increase is delayed by approximately 3 seconds. Overall, the results are good, although the peak power prediction is inconsistent between the three cases.

#### CONCLUSIONS AND FUTURE WORK

The results here indicate that the spatial kinetics option in RELAP5 is capable of analyzing the core behavior during a control rod ejection and rod withdrawal transients. The discrepancies that occur between the RELAP5 result and the reference can be attributed to differences in data or in core modeling approximations

Future work will include the BWR stability benchmark calculations specified by NEACRP.

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- 5 H. Finnemann, et. al., "Results of LWR Core Transient Benchmarks," Proceeding Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications, Vol. 2, p. 243, Kernforschungszentrum, Karlsruhe, April, 1993.

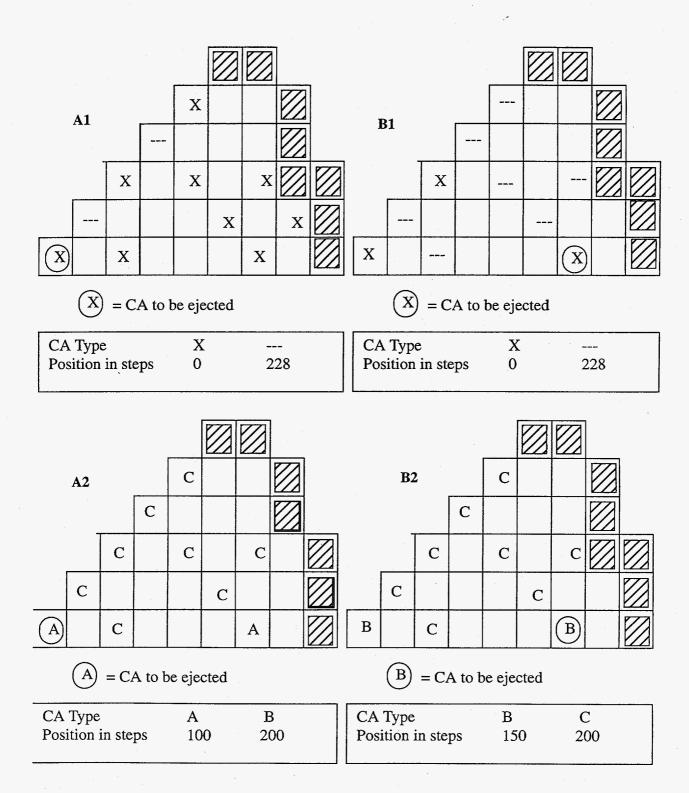


Figure 1. Initial Core Configuration for Series A and B Rod Ejection Transients.

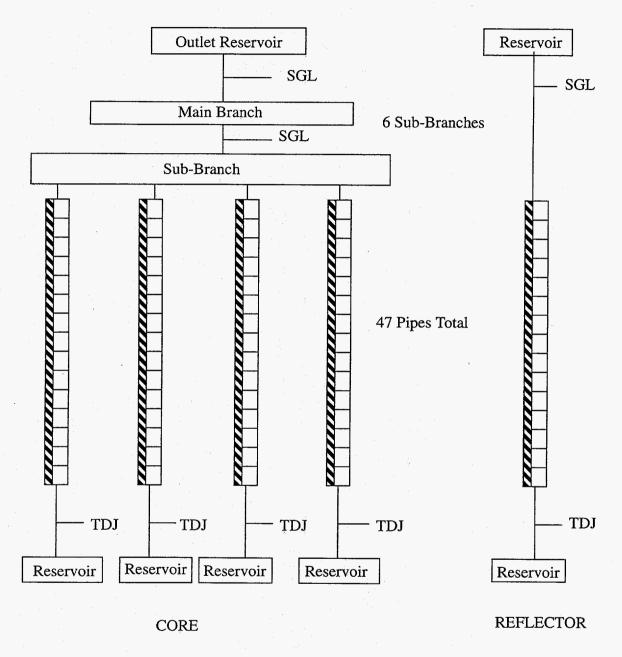
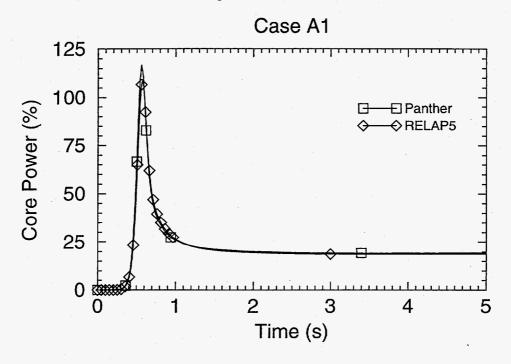


Figure 2. RELAP5 Model for NEACRP PWR Kinetics Benchmark Problem.

## NEACRP Ejected Rod Benchmark



## NEACRP Ejected Rod Benchmark

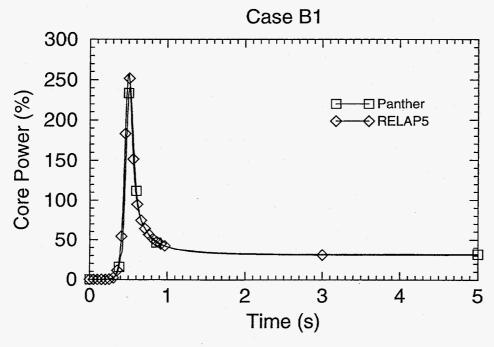
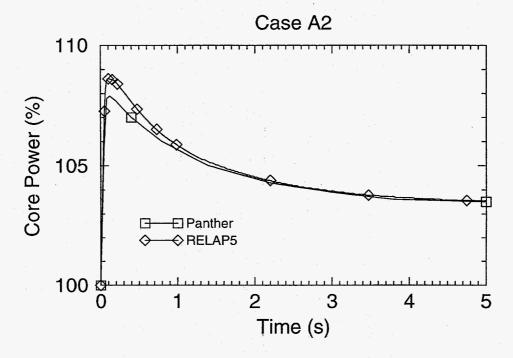


Figure 3. Transient Core Power for Rod Ejection from Hot Zero Power.

# NEACRP Ejected Rod Benchmark



# NEACRP Ejected Rod Benchmark

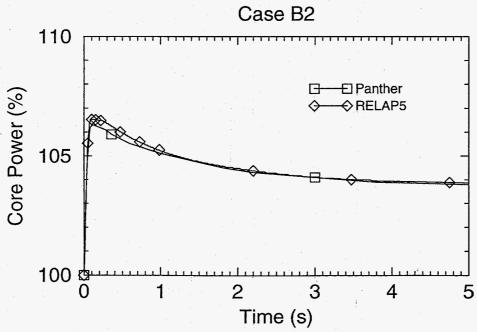


Figure 4. Transient Core Power for Rod Ejection from Hot Full Power.

### **NEACRP Rod Withdrawal Benchmark**

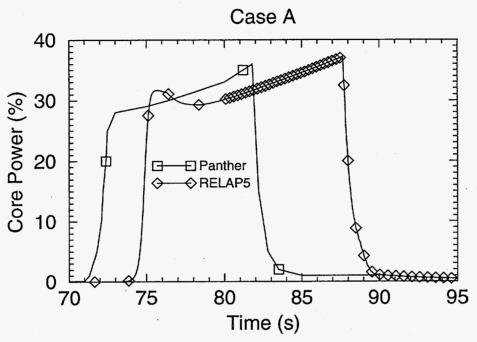


Figure 5. Transient Core Power for Rod Withdrawal Case A.

## **NEACRP Rod Withdrawal Benchmark**

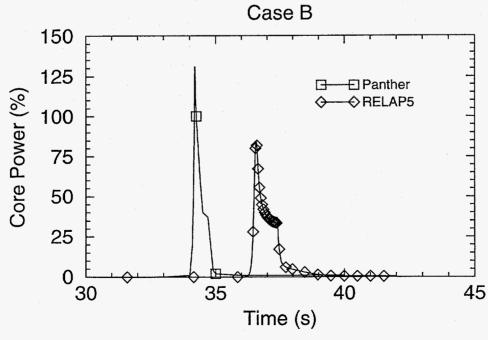


Figure 6. Transient Core Power for Rod Withdrawal Case B.

## **NEACRP Rod Withdrawal Benchmark**

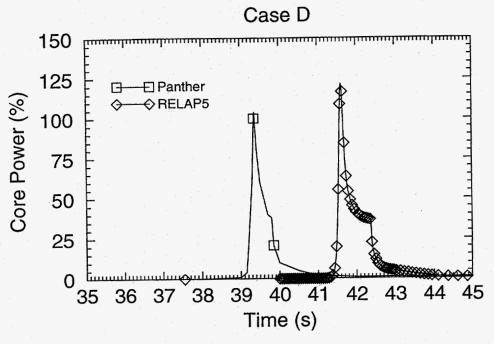


Figure 7. Transient Core Power for Rod Withdrawal Case C.

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