NUREG/CR-1823
EGG-CAAP-5217

Description and Characterization of Evaluation Models in FRAPCON-1

Manuscript Completed: August 1980
Date Published: December 1980

Prepared by
E. T. Laats, R. Chambers

EG&G Idaho, Inc.
Idaho Falls, ID 83415

Prepared for
Division of Systems Integration
Office of Nuclear Reactor Regulation
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
NRC FIN A6167

ABSTRACT

A preliminary set of nine evaluation models to obtain thermal conservatism in fuel rod behavior calculations was added to the FRAPCON-1 computer code, a code used to calculate fuel rod behavior in a nuclear reactor during steady-state operation. Checkout and characterization of the evaluation models were performed, and conclusions were reached concerning their correctness of coding and relative performance for providing thermal conservatism.

NRC FIN NO. A6167 - INEL Fuel Performance Code Program

SUMMARY

A preliminary set of nine evaluation models (EMs) was added to the FRAPCON-1 computer code used to calculate fuel rod behavior in a nuclear reactor during steady-state operation. The intent was to provide an audit code to be used in the United States Nuclear Regulatory Commission (NRC) licensing activities when calculations of conservative fuel rod temperatures are required. The EMs place conservatisms on the calculation of rod temperature by modifying the calculation of rod power history, fuel and cladding behavior models, and materials properties correlations.

The correctness of the models' coding was checked by performing a series of runs, each run using a single different EM, and by comparing the EM code calculations with a best-estimate calculation. Results indicate that the EMs were coded properly and operated as expected.

A sensitivity study was then performed to determine relative model importance and model interactions when more than one EM was used simultaneously. Results indicate that nearly all combinations of EMs used simultaneously produced thermal conservatism in the calculations. The combinations of EMs that maximized thermal conservatism were identified as well as combinations that produced nonconservative calculations.

The entire set of EMs was deemed as a reasonable first attempt to produce an audit code that would calculate conservative fuel rod temperatures. However, areas of deficiency were identified in the models' failure to adopt mechanistic modeling of these fuel behavior phenomena, in lieu of the high state-of-the-art of understanding these mechanisms.

ACKNOWLEDGMENTS

The authors wish to acknowledge the two people who provided major contributions during the task. G. A. Berna provided continuous model development support and is credited as author of the evaluation model description presented in this report. J. C. Voglewede of the USNRC Core Performance Branch assisted in providing the evaluation model specifications and in guiding the implementation of these models.

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DESCRIPTION AND CHARACTERIZATION OF EVALUATION MODELS IN FRAPCON-1

1. INTRODUCTION

In 1977, the United States Nuclear Regulatory Commission (NRC) developed a plan to coordinate several NRC-funded fuel behavior modeling programs to improve utilization of existing efforts. The first major product is the new NRC steady-state best-estimate (BE)/evaluation model (EM) fuel behavior code, FRAPCON-1. The BE portion of FRAPCON-1 was composed of the existing NRC codes FRAP-S3[1] and GAPCON-Thermal-3.[2] Code fabrication was completed in November 1978,[3] and a thorough assessment of BE code capabilities was completed in 1979.[4] A parallel effort to develop the conservative EMs for FRAPCON-1 was also conducted.[5] A preliminary set of nine EMs was approved by the NRC for FRAPCON-1 and were recently incorporated into the code. The documentation and characterization of the EMs are the subjects of this report.

The nine EMs approved for FRAPCON-1 by the NRC cover the areas of rod power history, fuel and cladding behavior models, and materials properties correlations. A two part characterization of these models was conducted. First, a series of FRAPCON-1 cases were run in which each model was used one at a time. Second, a sensitivity study was performed to determine the relative influence and importance of each EM and to determine the effects of EM interactions upon the calculations.

A description of the EMs is presented in Section 2. Performance characteristics of the individual EMs are given in Section 3, and the results of the sensitivity study are discussed in Section 4. The conclusions and recommendations are discussed in Section 5. Variables included in the FRAPCON-1 input deck for the Zion-1 test case used in the characterization study are briefly described in Appendix A. The special input requirements to use the EMs in FRAPCON-1 are listed in Appendix B.

2. DESCRIPTION OF EVALUATION MODELS

The preliminary set of nine evaluation models have been included in FRAPCON-1 to provide a conservative calculation of fuel rod temperature predictions. These EMs fulfill 10 CFR Part 50, Appendix K criteria[6] for predicting the steady-state fuel temperatures and stored energy in a nuclear reactor prior to a loss-of-coolant accident.

The nine EMs in FRAPCON-1 are:

1. The input rod power must be based on continuous operation at maximum core power with maximum peaking factors and appropriate uncertainties considered. No credit is given for gamma heating and gamma smearing. The code does not apply a multiplier to the input rod power; all peaking factors are to be included in the input power. The only action taken by FRAPCON-1 to fulfill this requirement is to print a message to the code user which states the above specifications.

2. Fuel dimensional changes include fuel swelling, densification, thermal expansion, and relocation. Restructuring is not considered. The fuel is treated as incompressible for mechanical response calculations. No modifications to FRAPCON-1 were needed to fulfill this specification. Its intent is to ensure that any future code versions do not exclude the presently modeled sources, or add other sources, of fuel geometry changes.

3. The fuel densification EM is specified in Reference 7. The fuel pellet diametral strain due to densification is determined by the following model:

$$\Delta d = \frac{-Dr}{3\ \rho}$$

where

Δd	=	change in pellet diameter due to densification (in.)
ρ	=	initial fuel density (g/cm^3)
Dr	=	$0.5\ (\rho_r - \rho)\ \log_{10}\ (BU/20)$, if $(\rho_r - \rho) \leq 0.4384$ (when BU is less than 20, Dr is set to zero and if burnup is greater than 2000, BU is set to 2000)
	=	$0.5\ (\rho_r - \rho)\ \log_{10}\ (BU/5)$, if $(\rho_r - \rho) > 0.4384$ (when BU is less than 5, Dr is set to zero and if burnup is greater than 500, BU is set to 500)
ρ_r	=	fuel resintered density (g/cm^3)
BU	=	local burnup (MWd/tU).

4. The fuel relocation EM is taken from Reference 8. The model is

$$\Delta_{EM} = \Delta_{BE} - 0.28\ \delta$$

where

Δ_{EM}	=	EM fuel surface relocation (in.)
Δ_{BE}	=	fuel surface relocation (in.) given below
δ	=	as-fabricated gap (in.).

The BE model is

$$\Delta_{BE} = 40.0 \left[\frac{B}{1 + B} + 0.8P + 1 \right] \frac{\delta}{100.0}$$

where

$B = \exp(-4.0 + BU^{1/4})$

P = local power (kW/ft)

BU = local burnup (MWd/tU).

5. The cladding dimensional changes account for only elastic deformation and thermal expansion. No plastic deformation or creepdown is allowed. Henceforth, for brevity, this EM is called the "no cladding creepdown EM."

6. The pellet-to-cladding gap conductance EM is based on the uniform annular gap model of FRAPCON-1. No credit is given for pellet-cladding interfacial pressure while the gap is closed.

7. The fuel thermal conductivity EM is based on an integrated thermal conductivity value of 93 W/cm for fuel of 95% theoretical density. The integration represents the temperature range from 273 K to UO_2 melting temperature. The EM is a function of temperature and local density. No adjustment is made to account for pellet cracking effects.

8. The fuel stored energy EM specifies the reference temperature to be 273 K when calculating the amount of stored energy. FRAPCON-1 otherwise uses 298 K.

9. The fission gas release EM is the MacDonald-Weisman model, described in Reference 3, with a release acceleration applied when the local rod burnup exceeds 1.73×10^6 MWs/kg (20,000 MWd/tU). The gas release fraction as presented in Reference 9 is given as

$$F' = F + (1 - F)Y$$

where

F' = accelerated gas release fraction

F = gas release fraction computed by MacDonald-Weisman model [if BU is less than 20,000, then F is determined at current fuel temperature and burnup and if BU is greater than or equal to 20,000, then F is determined at current fuel temperature and at burnup equal to 1.73×10^6 MWs/kg (20,000 MWd/tU); a minimum value for F of 1% release is enforced when the rod burnup exceeds 1.73×10^6 MWs/kg]

$$Y = \frac{1 - \exp[-0.0000436\ (BU-20{,}000)]}{1 + (0.665/F)\exp[-0.0001107\ (BU-20{,}000)]}$$

BU = burnup (MWd/tU).

In FRAPCON-1, the fraction of gas released applies to the amount available for release at a given time step at each axial and radial node, not to the total amount produced in the rod. This modeling approach can produce an apparent overconservatism if improperly interpreted.

3. EVALUATION MODEL CHECKOUT

To ensure proper coding of the EMs, a one-at-a-time model checkout was performed. Nine cases were run, each case using a different EM. The basic input deck was best-estimate and represented the irradiation of a core lead rod to about 2.8 x 10^6 MWs/kg burnup in the Zion-1 commercial reactor. The input deck was assembled primarily from information presented in safety analysis reports. If required input data were not available, then best-estimate values were used. The power history consis d of steady-state operation at a peak power level of 49 kW/m, with startup ramps at beginning-, middle-, and end-of-life. Other variables included in the input deck are described in Appendix A. A description of the EM input requirements is presented in Appendix B.

The results of this checkout were divided into three groups. First, when using either of the first two EMs (which list the rod power and fuel pellet geometry considerations), the code prints an appropriate message in the problem input listing. Otherwise, as expected, the calculations were identical to the BE calculations. Second, using the stored energy EM produced a constant increase of the calculated stored energy, as compared to the BE values. Again, this trend was expected. And last, at some time during the Zion-1 irradiation history, each of the six remaining EMs produced calculated temperatures and stored energies that were greater than those predicted by the best-estimate models. Calculated temperatures and stored energies greater than the best-estimate values are called "conservative" values henceforth. None of the EMs produced conservatism during the entire irradiation history. During the beginning-of-life (BOL) ramp, only the fuel relocation EM and the fuel thermal conductivity EM by themselves produced conservative values. All other EMs had no effect. The BOL temperature and stored energy ramps are shown on Figures 1 through 4. These figures compare the EM and the BE FRAPCON-1 calculations. On Figure 1, all fuel centerline temperature curves essentially overlay. On Figure 2, the temperature curve for the fuel thermal conductivity EM is below the BE curve for power levels between 3 and 30 kW/m. However, these EM calculations are still thought to be conservative. The BE calculations

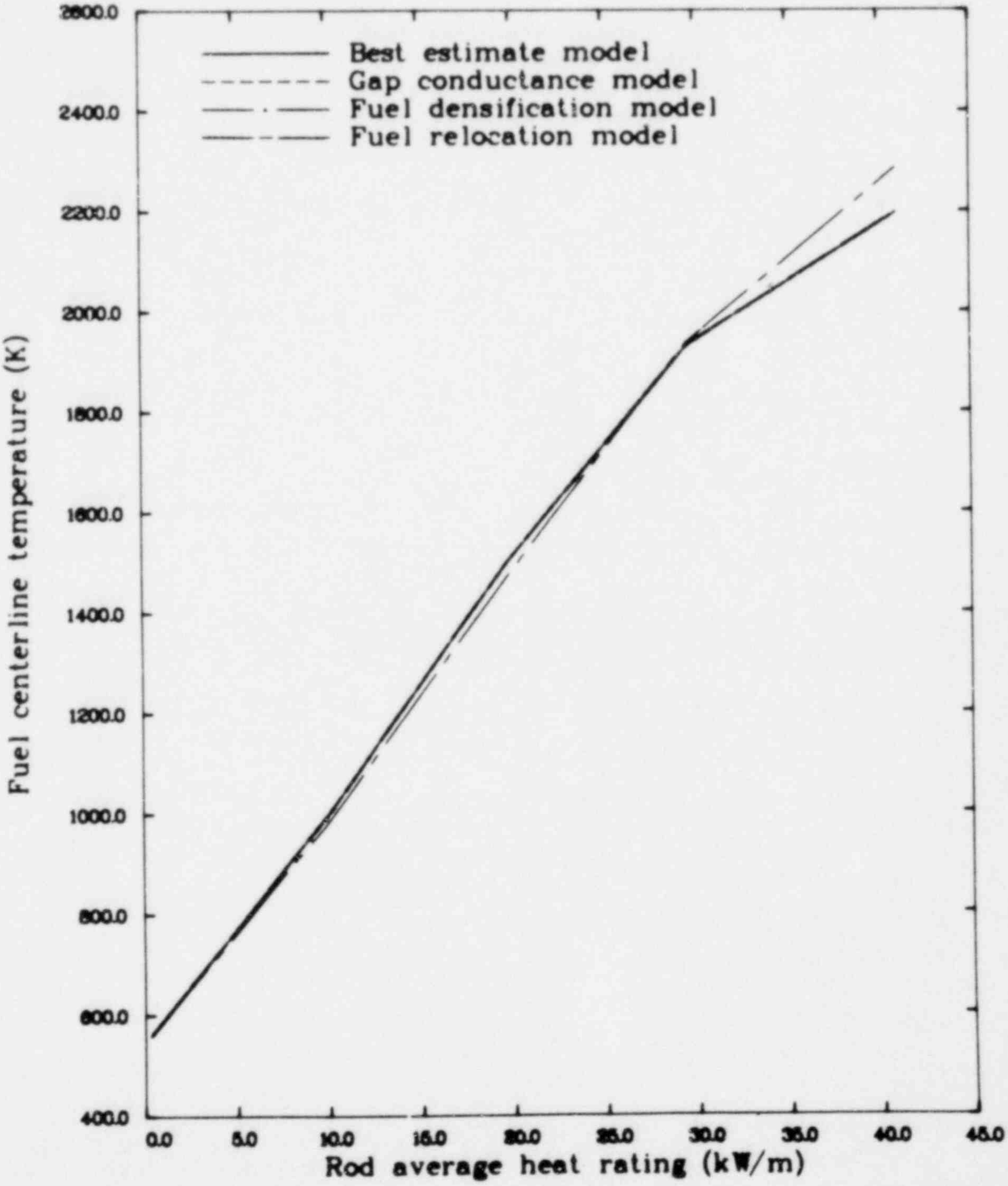

Figure 1. Fuel centerline temperature during beginning-of-life ramp using gap conductance, densification, or relocation evaluation models.

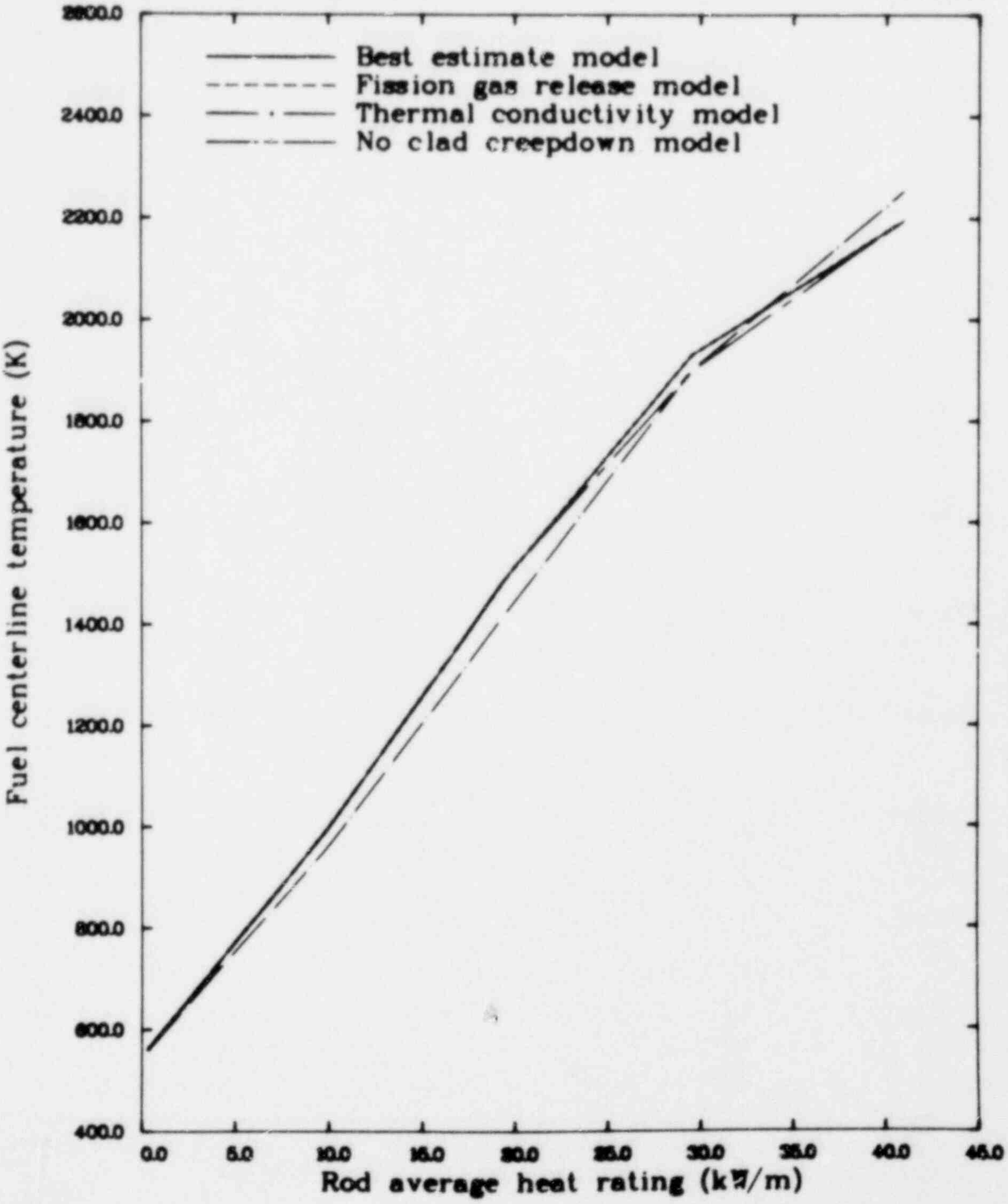

Figure 2. Fuel centerline temperature during beginning-of-life ramp using gas release, thermal conductivity, or creepdown evaluation models.

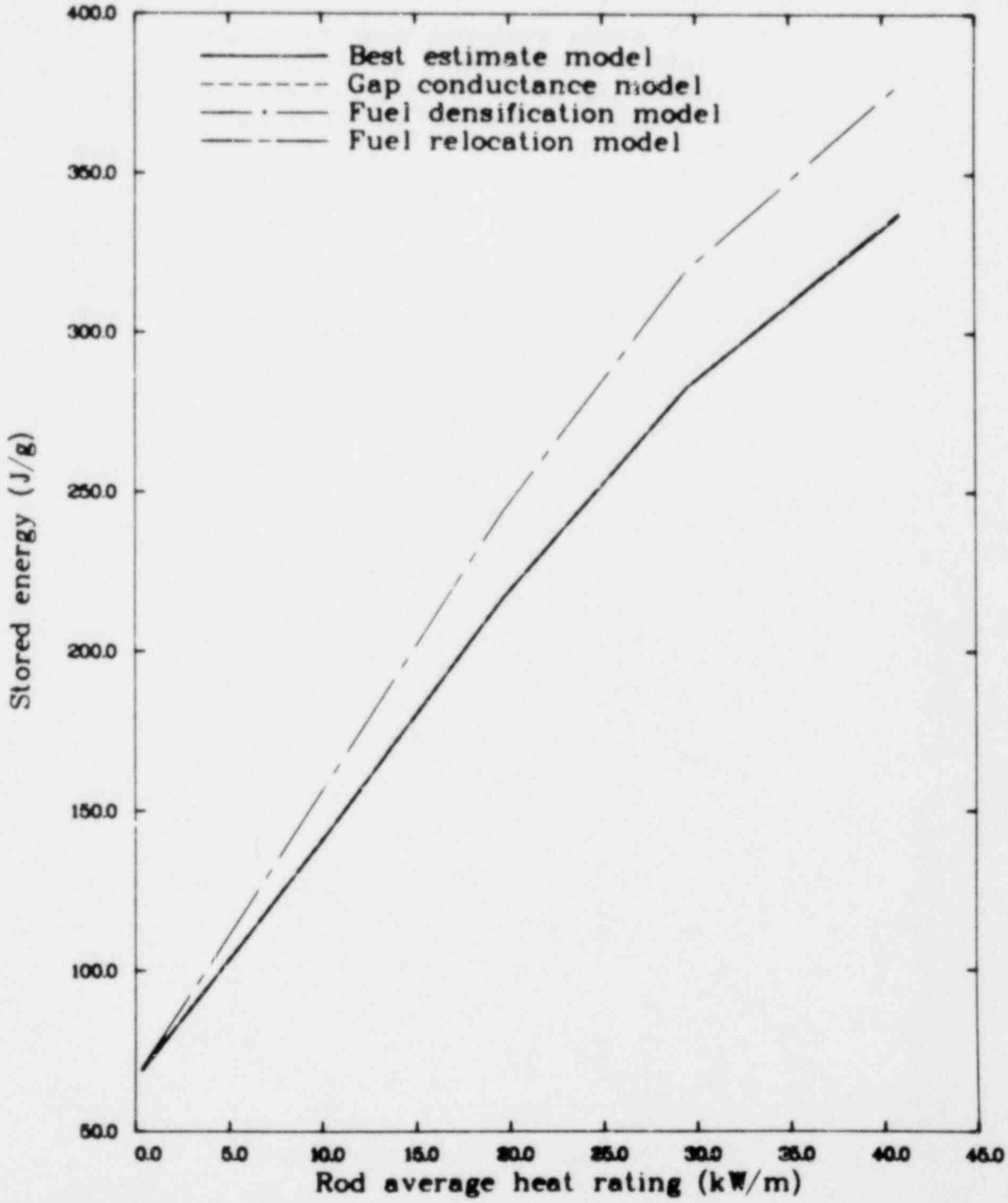

Figure 3. Stored energy during beginning-of-life ramp using gap conductance, densification, or relocation evaluation models.

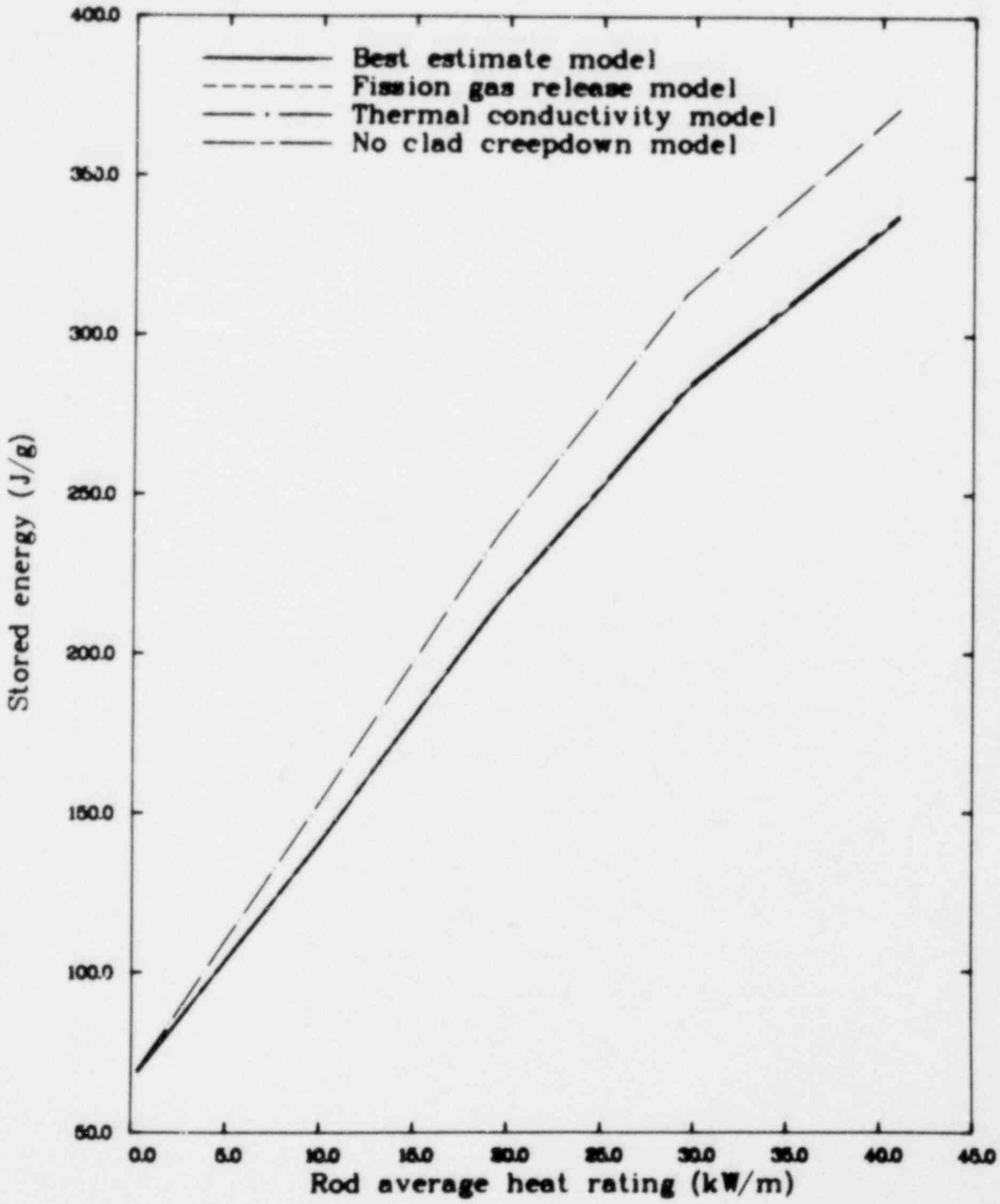

Figure 4. Stored energy during beginning-of-life ramp using gas release, thermal conductivity, or creepdown evaluation models.

have been characterized in Reference 4 as being overpredictive of the experimental data. The extent of the overprediction is 8% at 1500 K, on the average. Since the EM curve for fuel thermal conductivity is less than the BE curve by only 4%, the EM curve can be viewed as being conservative with respect to the data base used to assess FRAPCON-1. In contrast, the EM calculated values for stored energy, shown on Figures 3 and 4, are always conservative when either the fuel relocation or fuel thermal conductivity EMs are used.

Figures 5 through 12 show the calculated rod behavior during full-power steady-state operation (49 kW/m). The fuel centerline temperature histories are shown on Figures 5 and 6, the stored energy histories are shown on Figures 7 and 8, the cladding strain histories are shown on Figures 9 and 10, and the fuel rod internal pressure histories on Figures 11 and 12. The temperature and stored energy histories illustrated on Figures 5 through 8 show essentially identical trends. The fuel relocation and fuel thermal conductivity EMs are again the most influential BOL models. Soon after BOL, the fuel densification and cladding creep EMs produce significant changes from BE. The curve for the cladding creep EM remains conservative throughout the irradiation history, while the curves for fuel densification and fuel relocation approach and essentially replicate the best-estimate curve during the last half of the irradiation period. The curve for the fuel thermal conductivity EM is conservative until end-of-life (EOL), when the pellet-to-cladding gap has become very small from fuel swelling and cladding creepdown. As expected, the fission gas release and gap conductance EMs do not become effective until late in the irradiation period. Both EMs always produce conservative calculations.

Since the primary intent of implementing these EMs was to increase the conservatism of FRAPCON-1 thermal calculations, the effect upon strain and internal pressure was considered to be second order. As a result, the calculated strains and pressures are dependent upon the nature of the individual EM, and may or may not be greater than the BE values. All in all, the expected trends are observed in Figures 9 through 12. The fuel densification, cladding creep, and fuel relocation EMs are calculating

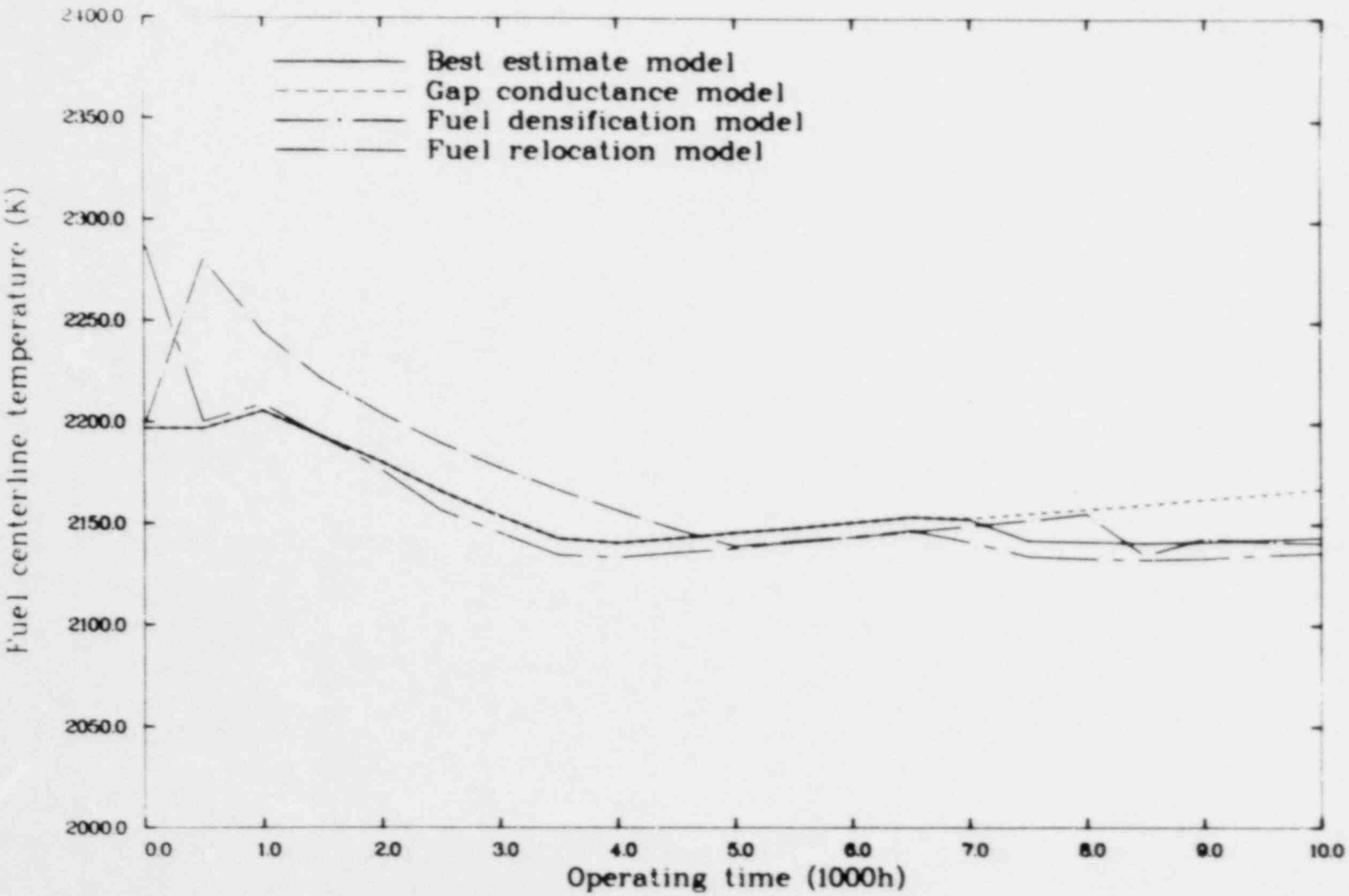

Figure 5. Fuel centerline temperature history using gap conductance, densification, or relocation evaluation models.

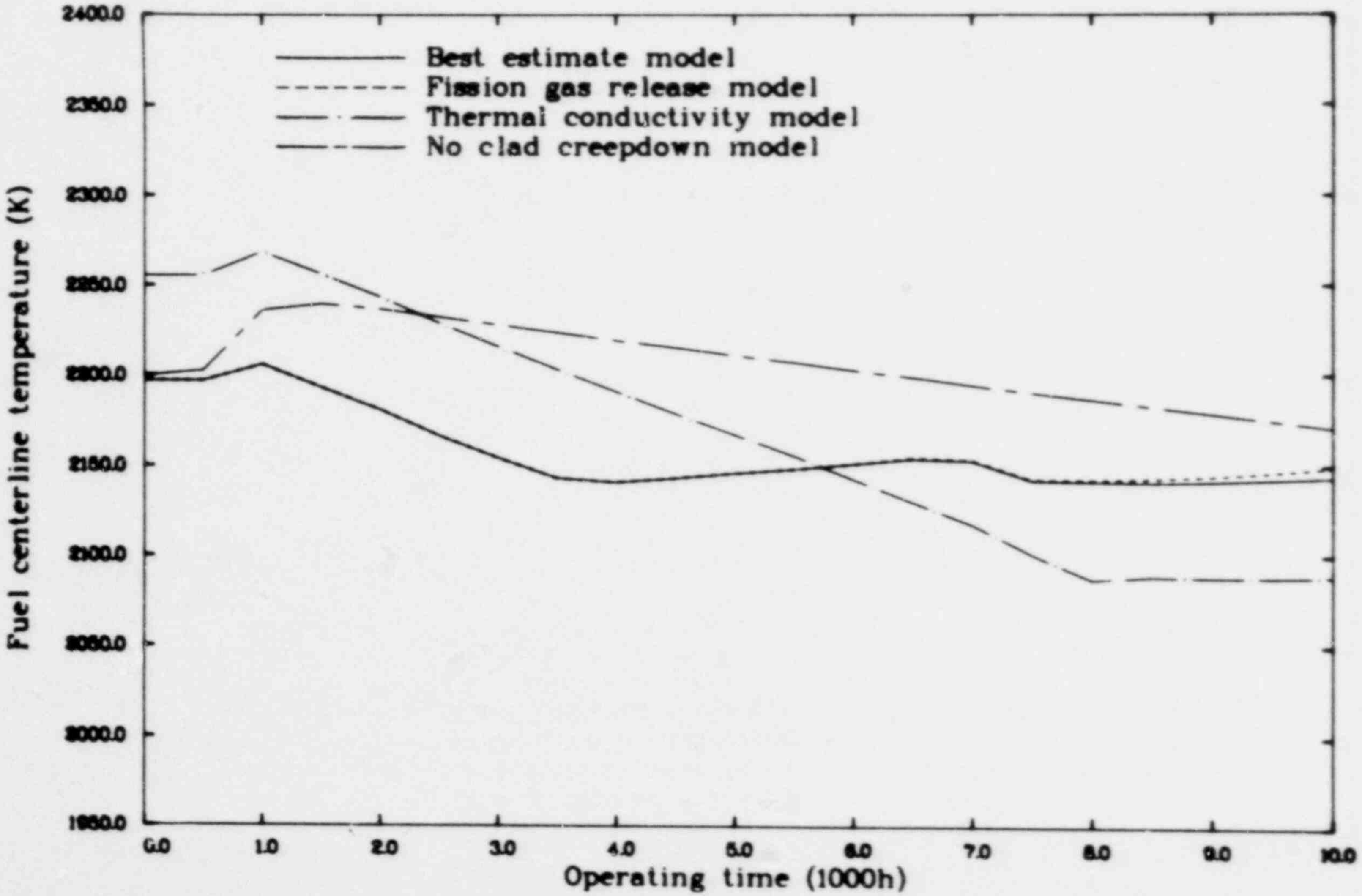

Figure 6. Fuel centerline temperature history using gas release, thermal conductivity, or creepdown evaluation models.

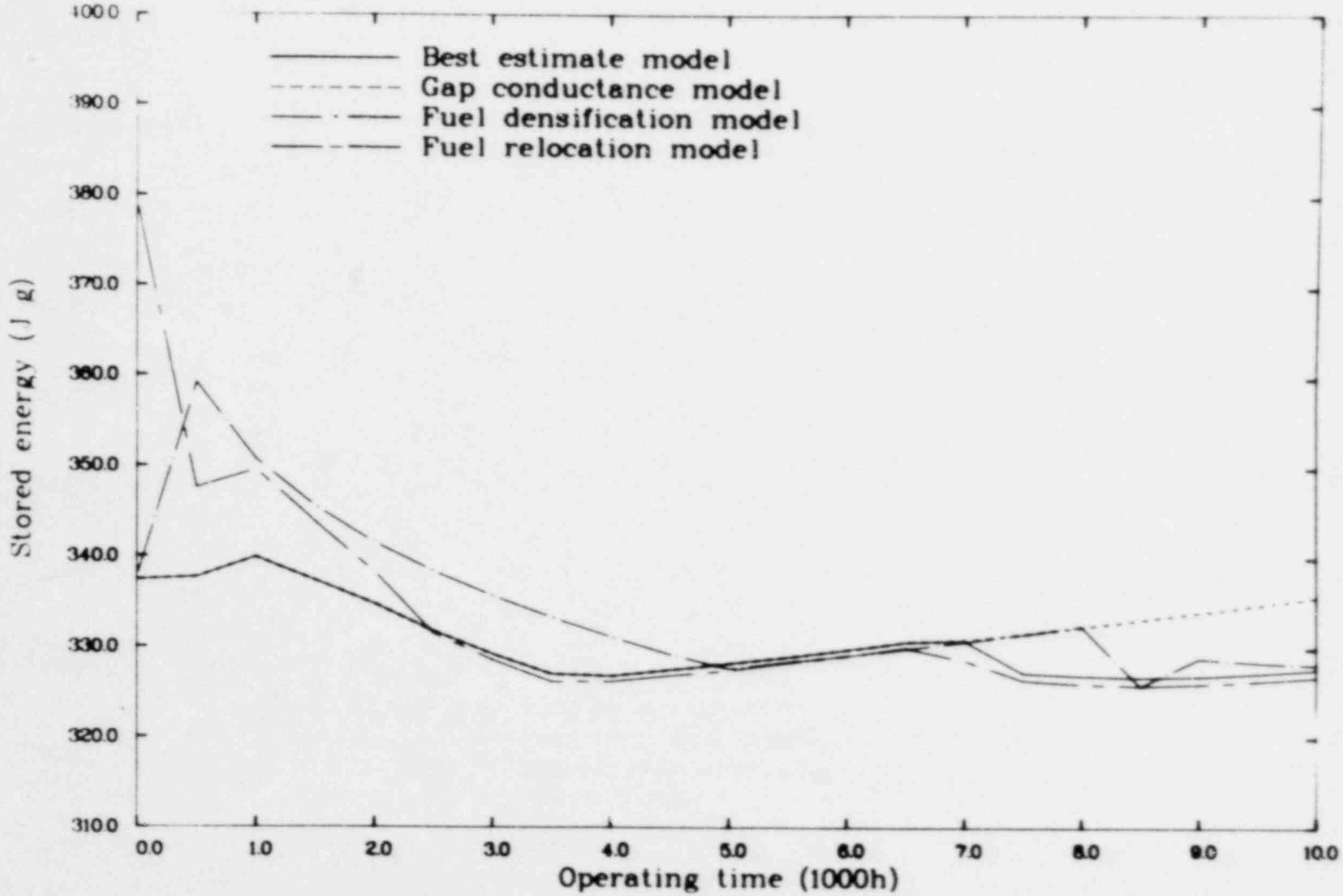

Figure 7. Stored energy history using gap conductance, densification, or relocation evaluation models.

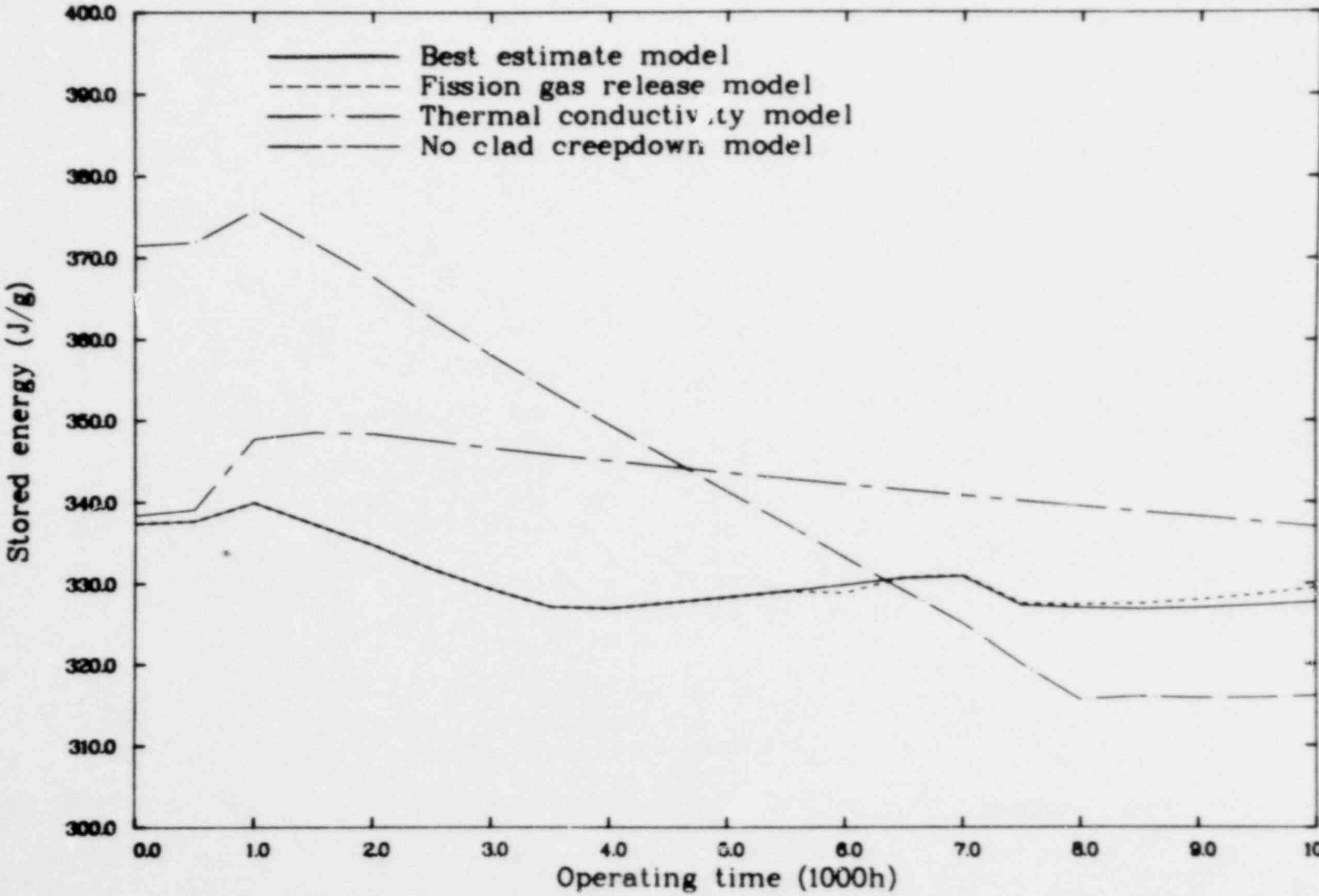

Figure 8. Stored energy history using gas release, thermal conductivity, or creepdown evaluation models.

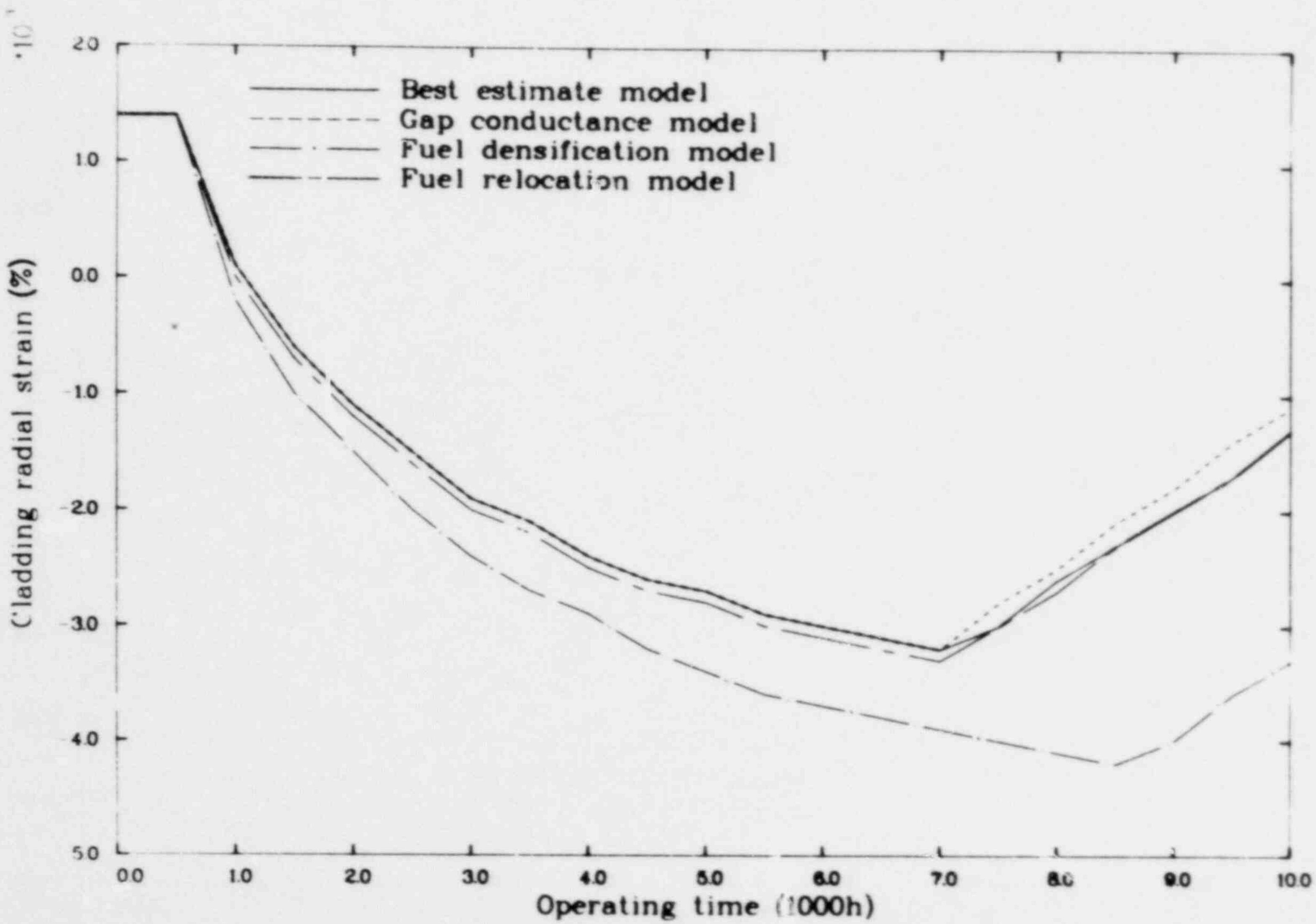

Figure 9. Cladding radial strain history using gap conductance, densification, or relocation evaluation models.

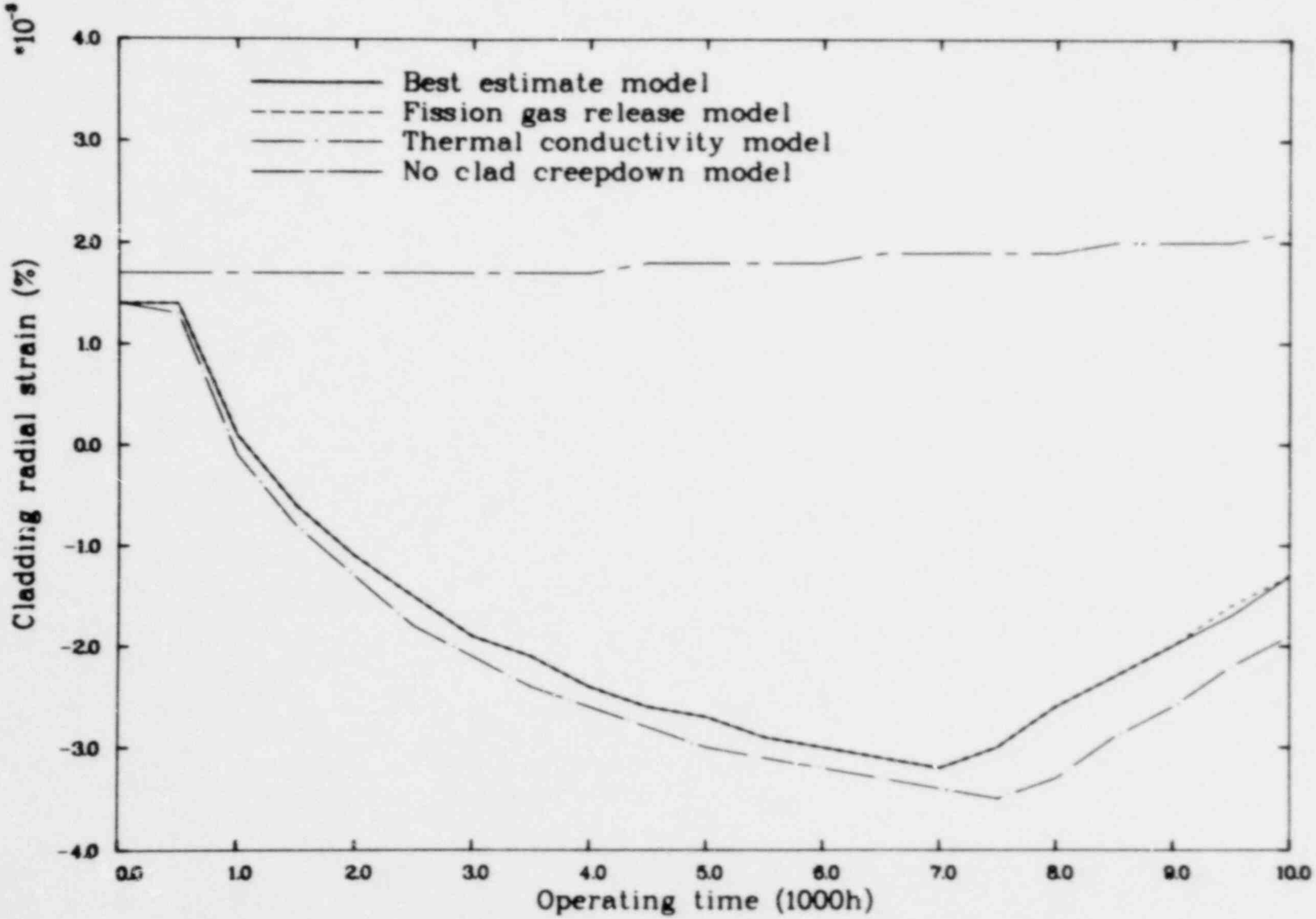

Figure 10. Cladding radial strain history using gas release, thermal conductivity, or creepdown evaluation models.

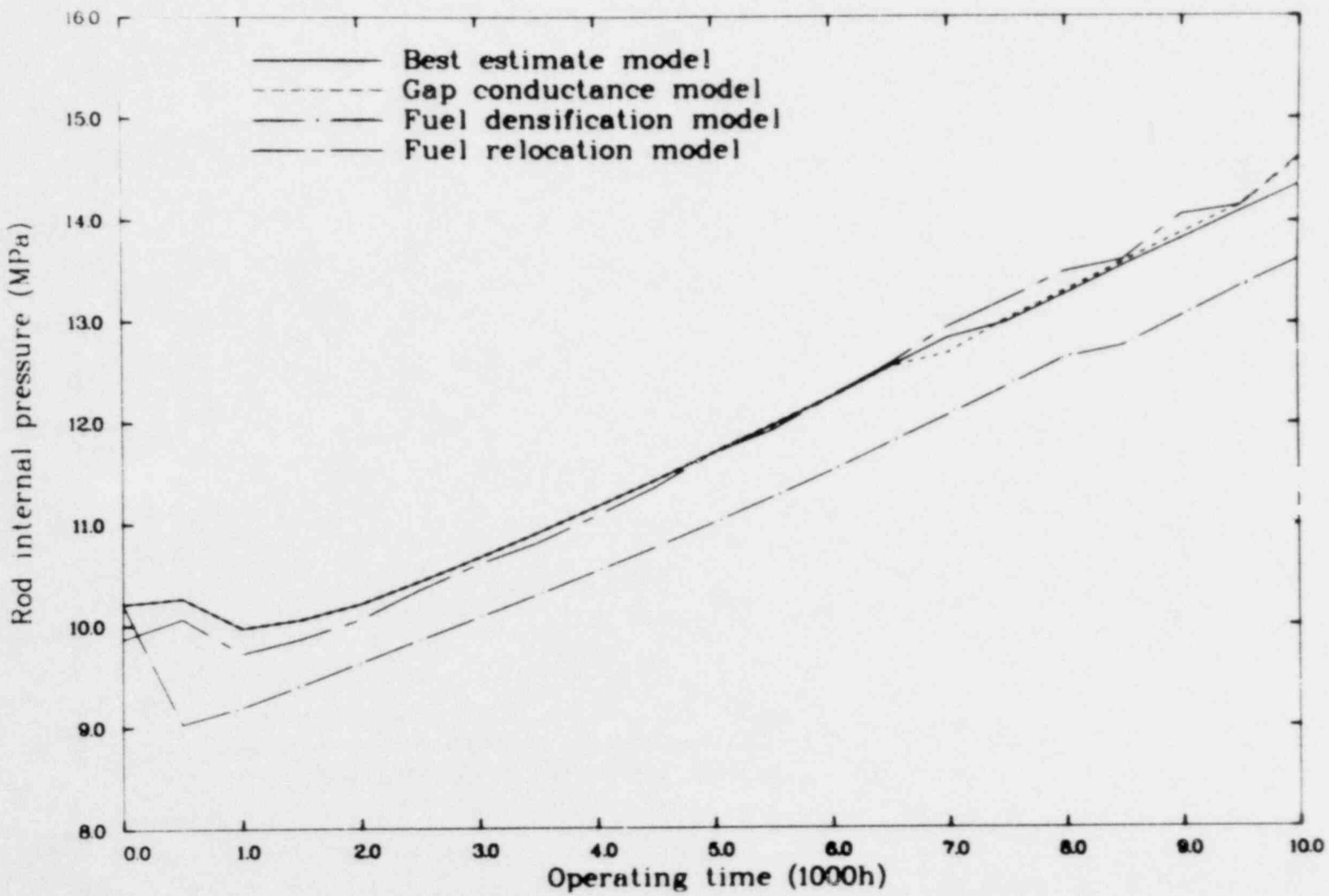

Figure 11. Rod internal pressure history using gap conductance, densification, or relocation evaluation models.

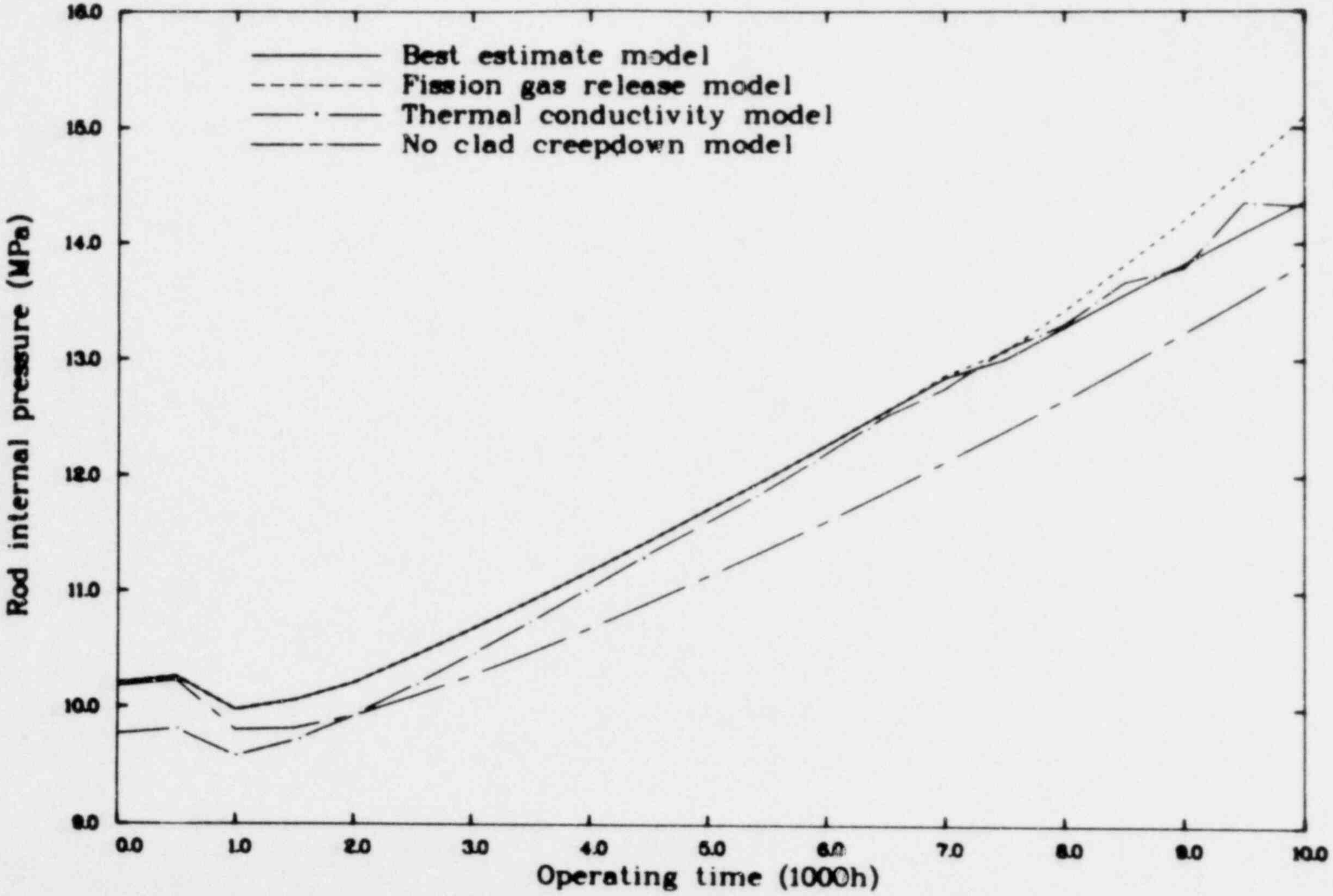

Figure 12. Rod internal pressure history using gas release, thermal conductivity, or creepdown evaluation models.

larger than best-estimate pellet-to-cladding gap sizes, thus providing a large internal void and lower than BE internal pressures. Late in life, the gas release EM is releasing fission gas at accelerated rates, thus increasing internal pressure, but effectively not altering the strain history. Also late in life, the gap conductance model is enhancing pellet-to-cladding interaction through higher fuel temperatures, producing smaller void volumes and higher internal pressures.

Examining all calculations shown in Figures 1 through 12, the EMs appear to have been coded properly and operating as expected.

4. SENSITIVITY STUDY RESULTS

To determine the relative influence of the FRAPCON-1 EMs upon fuel behavior calculations, a sensitivity study was conducted. As stated in the previous section, three of the nine EMs provide either input or model specifications, or set the reference temperature for stored energy calculations. The remaining six EMs were intended to add thermal conservatism through model changes. These six EMs are the subject of this study.

Used in this study were the fuel densification EM, the fuel relocation EM, the cladding deformation EM, the pellet-to-cladding gap conductance EM, the fuel thermal conductivity EM, and the fission gas release EM. Response surface methodology, as described in Reference 10, was used to determine the relative importance of each EM, and the interaction of using more than one EM simultaneously. The procedure is well developed and partially automated, and is relatively inexpensive when compared with other techniques such as Monte Carlo. Basically, the procedure consisted of four parts. First, a best-estimate input deck was fabricated to represent the irradiation of a core lead rod to about 2.8×10^6 MWs/kg burnup in the Zion-1 commercial reactor. This deck is identical to the Zion-1 deck described in the previous section and listed in Appendix A. Second, a series of runs were made in which the EMs were systematically turned off or on, as specified by the experiment design matrix. To assure a high degree of resolution, while maintaining a minimum number of runs, a one-fourth fractional factorial foldover design was used that resulted in a total of 16 runs (cases) being required with various off-on combinations of the EMs. The combinations of EMs used in each of the 16 cases are listed in Table 1. Third, the results of these 16 cases were processed by the automated uncertainty analysis program described in Reference 11. And fourth, interpretation of the results was performed.

For each of the 16 sensitivity study cases, the fuel centerline temperature and stored energy histories are shown on Figures 13 and 14. Examining these figures, two basic trends can be noted. Namely, the best-estimate calculation does not produce the minimum fuel centerline

TABLE 1. OPTIONS USED FOR EACH SENSITIVITY STUDY CASE

	EM Options Used					
Case	Fuel Thermal Conductivity	Gap Conductance	Fuel Relocation	Fuel Densification	No Cladding Creepdown	Fission Gas Release
1	X[a]	X	X	X	X	X
2		X	X			X
3	X		X		X	
4			X	X		
5	X	X		X		
6		X			X	
7	X					X
8				X	X	X
9						
10	X			X	X	
11		X		X		X
12	X	X			X	X
13			X		X	X
14	X		X	X		X
15		X	X	X	X	
16	X	X	X			

a. X indicates which EM was used for each case.

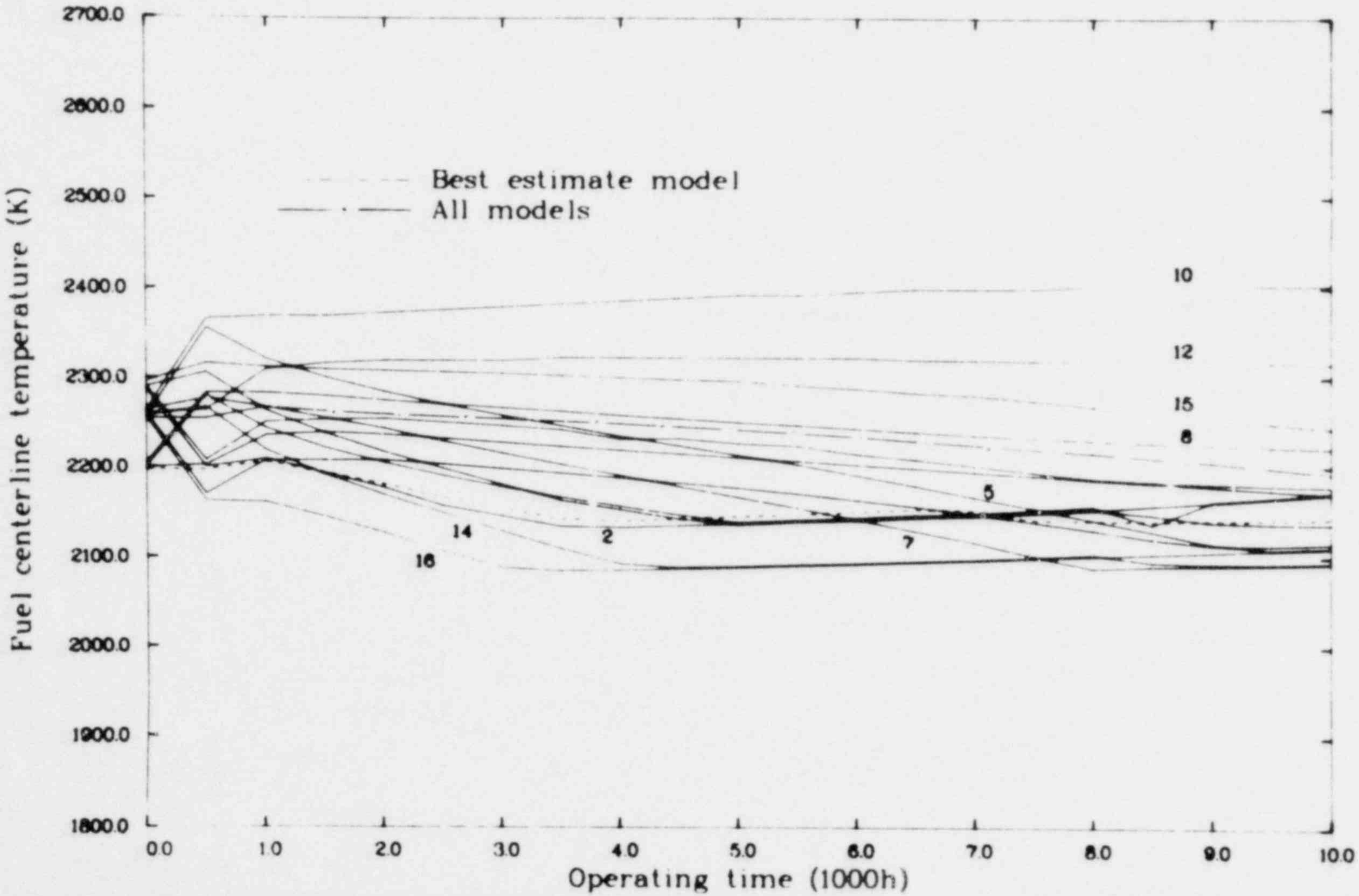

Figure 13. Fuel centerline temperature history for each sensitivity study case.

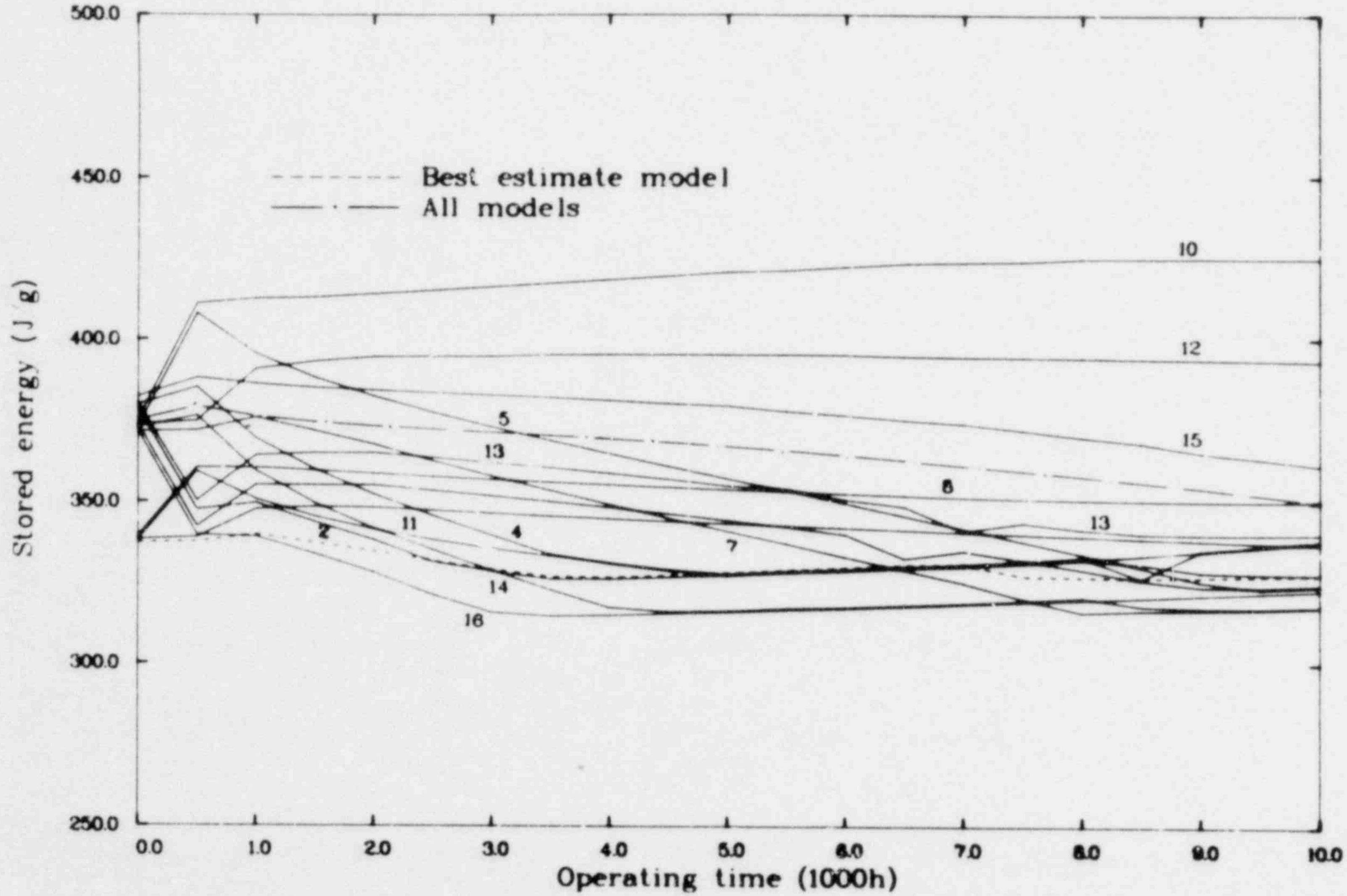

Figure 14. Stored energy history for each sensitivity study case.

temperature and stored energy histories. Also, the simultaneous use of all EMs does not provide the maximum conservatism. Since each of these EMs individually produce conservatism, these trends indicate that the effects of simultaneously using these EMs are neither additive nor multiplicative of the effect of the individual models, but rather some combination of additive and multiplicative. Upon examining the results of the sensitivity study analyses, the following conclusions were drawn:

1. All EMs were coded correctly.

2. The simultaneous use of all EMs considered in this study did produce conservative thermal calculations. However, the interactions among the various EMs are complicated, and, for a different problem, the EM code could conceivably produce nonconservative calculations at BOL.

3. The maximum perturbation from the best-estimate calculation was obtained by simultaneously using all EMs except the fuel relocation EM.

4. The most influential models were, in order of decreasing importance, the no cladding creepdown EM, the fuel thermal conductivity EM, the fuel densification EM, and the fuel relocation EM. The fission gas release and gap conductance EMs did provide a notable conservatism at high burnups, but the effect was small when compared with the effect of the other models.

5. Using the fuel thermal conductivity EM may or may not produce conservative thermal calculations. When used by itself or with any combination of the no cladding creepdown, densification, fission gas release or gap conductance EMs, the calculated thermal conditions are conservative. However, when used with the fuel relocation EM, the fuel centerline temperature and stored energy are reduced to the point of nonconservatism. The trend

results from a conflict between these two EMs. First, the fuel conductivity EM assumes that the fuel pellet is not cracked, thereby keeping the pellet conductivity relatively high when compared with the conductivity determined by the BE cracked pellet model. Second, the fuel relocation EM assumes the pellet does crack, thereby reducing the pellet-to-cladding gap and increasing the gap conductivity. Joint use of these EMs is physically unrealistic and produces the low temperatures and stored energies.

5. CONCLUSIONS AND RECOMMENDATIONS

Incorporating this preliminary set of nine evaluation models into FRAPCON-1 is a commendable first effort toward attaining a steady-state fuel behavior audit code. This code can be used to perform calculations which satisfy 10 CFR Part 50, Appendix K requirements if the code input requirements specified in Appendix B are fulfilled completely.

From the results of this analysis, the EMs are noted to be properly incorporated into FRAPCON-1 and are individually performing as expected. When more than one EM is used simultaneously, certain trends are noted. First, simultaneous use of all EMs did produce conservative thermal calculations. Second, maximum conservatism is attained when all but the fuel relocation EM are used simultaneously. Third, using only the fuel thermal conductivity and fuel relocation EMs together may produce nonconservative thermal calculations and thus should not be used. And fourth, the most influential EMs considered here are, in decreasing order of importance, the no permanent cladding deformation (no creepdown) EM, the fuel thermal conductivity EM, the fuel densification EM, and the fuel relocation EM.

Overall, the goal of attaining thermal conservatism has been achieved. However, more EM development should be pursued. The state-of-the-art of fuel rod behavior modeling has advanced to the point where physical mechanisms are understood fairly well and should be modeled to reflect current mechanism understanding. For example, the fuel thermal conductivity EM does not allow the effects of pellet cracking to influence the fuel conductivity calculation, but using the fuel relocation EM is intended to account for geometry changes due to pellet cracking. These models are physically inconsistent. Also, concerning the EM which does not allow cladding creepdown, the omission of creepdown is conservative, but unrealistic.[5] The rate of cladding creepdown has been characterized experimentally, and a conservative but realistic model should allow creepdown, within appropriate limits corresponding to statistical bounds on the experimental data.

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*Available for purchase from the NRC/GPO Sales Program, U.S. Nuclear Regulatory Commission, Washington, D.C. 20555, and the National Technical Information Service, Springfield, VA 22161

**Available for purchase from the National Technical Information Service, Springfield, VA 22161

APPENDIX A

INPUT VARIABLES FOR ZION-1 TEST CASE

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INPUT VARIABLES FOR ZION-1 TEST CASE

Variables included in the FRAPCON-1 input deck for the Zion-1 test case are listed in Table A-1.

TABLE A-1. INPUT VARIABLES FOR ZION-1 TEST CASE

Variable	Value
Cladding outside diameter	10.72 mm
Cladding inside diameter	9.48 mm
Pellet diameter[a]	9.29 mm
Pellet length	15.24 mm
Pellet density	95.0% of theoretical maximum
Fuel enrichment	2.8%
Fuel stack height	3.66 m
Plenum length	208.3 mm
System coolant pressure	15.51 MPa
Coolant inlet temperature	547 K
Peak rod power	49 kW/m

a. Pellets are dished.

APPENDIX B

INPUT REQUIREMENTS FOR USING EM VERSION OF FRAPCON-1

APPENDIX B

INPUT REQUIREMENTS FOR USING EM VERSION OF FRAPCON-1

Two input variables and a set of 10 evaluation model (EM) switches were added to FRAPCON-1 as part of the EM package. One input variable specifies the reference temperature (TREF) for the stored energy calculation and the second variable specifies the resintering density (RSNTR) for the fuel densification model. Of the EM switches, one (EMSWCH) is used to set all others on or off, or to specify that only some combination of the EM options is to be used. The reference temperature, densification, and EMSWCH options are described in Table B-1.

TABLE B-1. DESCRIPTION OF EMSWCH, RSNTER, AND TREF OPTIONS

Variable	Default Value	Description	Restriction and Options
EMSWCH	0	Evaluation model index	= 0 - No EM options used = 1 - All EM options used = -1 - User specifies options to be used
RSNTR	0.0 kg/m^3	Resintering density change	None
TREF	298 K	Reference temperature for stored energy	Greater than zero

If the third choice for EMSWCH is selected, the remaining nine EM switches are the input variables which are used to specify which EMs should be used. The input variables are given in Table B-2.

TABLE B-2. DESCRIPTION OF EM SWITCHES USED AS INPUT VARIABLES

Variable	Default Value	Description	Restriction and Option
EMPOWR	0	EM power required index	= 0 - Not assumed to be required = 1 - Assumed to be required and input appropriately
EMFUEL	0	EM fuel dimensional change index	= 0 - BE dimensional changes = 1 - EM dimensional changes
EMDENS	0	EM fuel densification index	= 0 - BE densification used = 1 - EM densification used[a]
EMRELO	0	EM fuel relocation index	= 0 - BE relocation used = 1 - EM relocation used
EMCLAD	0	EM cladding deformation index	= 0 - All deformation mechanisms included = 1 - No permanent deformation included
EMGAPC	0	EM gap conductance index	= 0 - BE gap conduction used = 1 - EM gap conduction used
EM93NC	0	EM fuel thermal conductivity index	= 0 - Thermal conductivity based on 97 W/cm = 1 - Thermal conductivity based on 93 W/cm and uncracked fuel
EMENRG	0	EM stored energy index	= 0 - Stored energy based on 298 K = 1 - Stored energy based on 273 K
EMFGAS	0	EM fission gas release index	= 0 - BE fission gas release used = 1 - EM fission gas release used

a. If this EM is used, also input a value for the RSNTR variable described in Table B-1 that is representative of the fuel rod being modeled.

The input cards described in Tables B-1 and B-2 follow a $EMFPCN card and are followed by a $END card. Again, the NAMELIST format is used. If EMSWCH = 0 or 1, these cards must be omitted.

NRC FORM 335
(7-77)

U.S. NUCLEAR REGULATORY COMMISSION

BIBLIOGRAPHIC DATA SHEET

1. REPORT NUMBER (Assigned by DDC)
NUREG/CR-1823

4. TITLE AND SUBTITLE (Add Volume No., if appropriate)
DESCRIPTION AND CHARACTERIZATION OF EVALUATION MODELS IN FRAPCON-1

2. (Leave blank)

3. RECIPIENT'S ACCESSION NO.

7. AUTHOR(S)
E. Thomas Laats and Rosanna Chambers

5. DATE REPORT COMPLETED
MONTH August | YEAR 1980

9. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code)
EG&G Idaho, Inc.
P. O. Box 1625
Idaho Falls, Idaho 83415

DATE REPORT ISSUED
MONTH January | YEAR 1981

6. (Leave blank)

8. (Leave blank)

12. SPONSORING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code)
Core Performance Branch
Division of Systems Integration
U. S. Nuclear Regulatory Commission
Washington, DC 20555

10. PROJECT/TASK/WORK UNIT NO.

11. CONTRACT NO.
FIN A6167

13. TYPE OF REPORT

PERIOD COVERED (Inclusive dates)

15. SUPPLEMENTARY NOTES

14. (Leave blank)

16. ABSTRACT (200 words or less)

A preliminary set of nine evaluation models to obtain thermal conservatism in fuel rod behavior calculations was added to the FRAPCON-1 computer code, a code used to calculate fuel rod behavior in a nuclear reactor during steady-state operation. Checkout and characterization of the evaluation models were performed, and conclusions were reached concerning their correctness of coding and relative performance for providing thermal conservatism.

17. KEY WORDS AND DOCUMENT ANALYSIS

17a. DESCRIPTORS

17b. IDENTIFIERS/OPEN-ENDED TERMS

18. AVAILABILITY STATEMENT
Unlimited

19. SECURITY CLASS (This report)
UNCLASSIFIED

20. SECURITY CLASS (This page)
UNCLASSIFIED

21. NO. OF PAGES

22. PRICE
$