NUREG/CR-1753-
PNL-3539

Application of Linear Propagation of Errors to Fuel Rod Temperature and Stored Energy Calculations

Prepared by M. E. Cunningham, A. R. Olsen, D. D. Lanning, R. E. Williford

Pacific Northwest Laboratory
Operated by
Battelle Memorial Institute

Prepared for
U.S. Nuclear Regulatory
Commission

NOTICE

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, or any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use, or the results of such use, of any information, apparatus product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights.

Available from

GPO Sales Program
Division of Technical Information and Document Control
U. S. Nuclear Regulatory Commission
Washington, D. C. 20555

and

National Technical Information Service
Springfield, Virginia 22161

Application of Linear Propagation of Errors to Fuel Rod Temperature and Stored Energy Calculations

Manuscript Completed: September 1980
Date Published: October 1980

Prepared by
M. E. Cunningham, A. R. Olsen, D. D. Lanning, R. E. Williford

Pacific Northwest Laboratory
Richland, WA 99352

Prepared for
Division of Reactor Safety Research
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
NRC FIN No. B2043

ACKNOWLEDGMENTS

The authors wish to acknowledge the sponsorship of Dr. W. V. Johnston and H. H. Scott of the Fuel Behavior Research Branch, U.S. Nuclear Regulatory Commission.

We would like to thank the following individuals from PNL: W. D. Bennett for her help with the computer graphics and C. M. Hagen and S. K. Edler for their editing assistance.

ABSTRACT

Linear propagation of errors evaluates modeling uncertainty by approximating a function of interest by first-order Taylor's series expansions and then approximating the variance of the function by the variance of the linear approximation. This report discusses uncertainty analysis for different nuclear fuel rod designs, the process of model validation, and the effect of cracked pellet fuel models upon temperature uncertainty.

Using a postulated power history, the uncertainty for the predicted thermal response of boiling water reactor (BWR) and pressurized water reactor (PWR) fuel rods was evaluated. Beginning-of-life (BOL) relative uncertainty for BWR and PWR fuel rods is approximately the same, while different end-of-life (EOL) thermal response results in different EOL uncertainty.

Determining the validity of modeling relative to reality is discussed in qualitative terms. Validity is dependent upon verifying that the code correctly implements the model and that satisfactory agreement is found between the model and measurements.

Fuel modeling codes are now using cracked pellet fuel models, which result in decreased fuel surface temperature. Estimated stored energy is lowered; but its relative uncertainty is increased. In general, however, the absolute upper uncertainty bound for stored energy is lower for a cracked pellet model than for a solid pellet model.

SUMMARY AND CONCLUSIONS

Linear propagation of errors (LPE) is being used by the Experimental Support and Development of Single-Rod Fuel Codes Program to evaluate both the uncertainties in fuel rod behavior and in the computer modeling of that behavior. This technique consists of approximating functions of interest by first-order Taylor's series expansions and then approximating the variance of the function by the variance of the linear approximation. When applied to an "abstract" (i.e., the basic models) of major fuel rod thermal performance codes, this method has been found to be adequate and useful in evaluating uncertainties for model predictions and the influence of various parameters. This report discusses predicted uncertainties for different fuel rod designs, provides a qualitative discussion on the process of model validation, and investigates the effect upon temperature uncertainty when using a cracked pellet fuel model.

A constant neutron flux power history was postulated for studying the predicted response of boiling water reactor (BWR) rod designs (7x7 and 8x8) and pressurized water reactor (PWR) rod designs (15x15 and 17x17). Plots of temperature, stored energy, and their associated uncertainties as a function of burnup are presented. Because of the fuel relocation model, temperatures decreased early in life with the result that the peak upper uncertainty bound for centerline temperature and stored energy occurred at beginning-of-life (BOL). The PWR rods maintain a constant temperature/power relationship after completion of fuel relocation while the BWR rods have an increasing thermal resistance. This difference is due to degradation of the fill gas thermal conductivity. The presence of more helium in prepressurized PWR rods helps to prevent degradation and maintains lower fuel temperatures.

Because fuel temperatures are highly dependent on power, parametric plots of centerline temperature and stored energy uncertainty as a function of linear heat rate uncertainty are presented. At BOL all rod designs have approximately the same relative uncertainty. At end-of-life (EOL), the difference in thermal performance between BWR and PWR rods results in differing relative uncertainties.

Determining the validity of modeling relative to reality is important from a safety standpoint. Three formal definitions are presented here:

- code verification - The process of verifying that a computer code implementation of a model or a set of models is done correctly.
- model analysis - The process of gaining an understanding of the theoretical model, often done with sensitivity analysis.
- model validation - The comparison of computer code output to data obtained from an observed physical situation.

A qualitative discussion of model development and validation is based around these three definitions. To illustrate points of the discussion, examples of model validation are included.

Models that better simulate the cracked nature of pellet fuel are currently being implemented in fuel thermal performance codes. These models change the predicted thermal behavior of fuel rods by decreasing the fuel surface temperature (because of fuel relocation closing the gap) and increasing the gap conductance, and by decreasing the effective fuel thermal conductivity because of the cracks. These changes affect the uncertainty analysis by reducing the assigned uncertainty on gap conditions and fuel surface temperature, while increasing the assigned uncertainty for fuel thermal conductivity. Thus, when comparing solid versus cracked model predictions for the same centerline temperature, the cracked pellet model results in a lower stored energy (because of lower volumetric average fuel temperature) and increased relative uncertainties for predicted centerline temperature and stored energy. Even though the cracked pellet model may have a higher relative uncertainty for stored energy its upper absolute bound is generally lower than that of the solid pellet model because of the lower predicted value for stored energy.

CONTENTS

ACKNOWLEDGMENTS	iii
ABSTRACT	v
SUMMARY AND CONCLUSIONS	vii
INTRODUCTION	1
BACKGROUND	3
LINEAR PROPAGATION OF ERRORS	3
APPLICATION OF LINEAR PROPAGATION OF ERRORS	6
ASSIGNMENT OF UNCERTAINTY	8
Local Linear Heat Rate	8
Gas Thermal Conductivity	9
Fuel Thermal Conductivity	9
Flux Depression	10
Specific Heat	10
SUMMARY OF PREVIOUS RESULTS	11
FUEL ROD DESIGN ANALYSIS	12
FUEL ROD TEMPERATURES	20
TEMPERATURE UNCERTAINTY	37
MODEL AND CODE VERIFICATION	45
MODELING AND REALITY	45
CODE VERIFICATION	49
MODEL ANALYSIS	50
MODEL VALIDATION	51
EXAMPLES OF VALIDATION	55
CRACKED PELLETS AND UNCERTAINTY ANALYSIS	65

REFERENCES	73
APPENDIX A: THERMAL MODELS IN STORE	A.1
APPENDIX B: THERMAL RESISTANCE	B.1
APPENDIX C: BURNUP DEPENDENT FILL GAS COMPOSITION	C.1

FIGURES

1	Interrelationships of Variables and Models in a Fuel Performance Code	7
2	Thermal History for BWR 7x7 (Case 1)	21
3	Thermal History for BWR 8x8 (Case 1)	22
4	Thermal History for BWR 8x8, 3 atm (Case 1)	23
5	Thermal History for PWR 15x15 (Case 1)	24
6	Thermal History for PWR 17x17 (Case 1)	25
7	Thermal History for BWR 7x7 (Case 2)	26
8	Thermal History for BWR 8x8 (Case 2)	27
9	Thermal History for BWR 8x8, 3 atm (Case 2)	28
10	Thermal History for PWR 15x15 (Case 2)	29
11	Thermal History for PWR 17x17 (Case 2)	30
12	Thermal History for PWR 17x17, 1 atm (Case 2)	31
13	Thermal Resistance History for Case 1	36
14	Thermal Resistance History for Case 2	36
15	Beginning-of-Life Relative Uncertainty for an LWR Rod at 20 kW/m	39
16	Beginning-of-Life Relative Uncertainty for an LWR Rod at 35 kW/m	39
17	Beginning-of-Life Relative Uncertainty for an LWR Rod at 50 kW/m	40
18	End-of-Life Relative Uncertainty for a BWR Rod at 20 kW/m	42
19	End-of-Life Relative Uncertainty for a BWR Rod at 35 kW/m	42
20	End-of-Life Relative Uncertainty for a BWR Rod at 50 kW/m	43
21	End-of-Life Relative Uncertainty for a PWR Rod at 20 kW/m	43
22	End-of-Life Relative Uncertainty for a PWR Rod at 35 kW/m	44
23	End-of-Life Relative Uncertainty for a PWR Rod at 50 kW/m	44
24	Components of Modeling Process	46

25	Computer Code Implementation of Theoretical Model	50
26	Verification of Steady-State Fuel Radial Temperature Profile Model	56
27	Validation of Gas Thermal Conductivity Model	57
28	Example of Validation of a Fuel Performance Code	58
29	Comparison of GAPCON-THERMAL-3 to IFA-513 Startup Data	62
30	Comparison of FRAPCON-1 to IFA-513 Startup Data	63
31	Minimum Conductivity Multiplier Values as a Function of Thermal Resistance	68
32	BWR 8x8 Stored Energy Based on Solid and Cracked Pellet Models .	72
33	BWR 8x8 Stored Energy Upper Absolute Uncertainty Bounds . . .	72
B.1	Components of Resistance	B.2
B.2	Resistance Behavior of Various Rods	B.2
C.1	Fill Gas Composition History for BWR 7x7, Case 2	C.2
C.2	Fill Gas Composition History for BWR 8x8, Case 2	C.2
C.3	Fill Gas Composition History for 3 atm BWR 8x8, Case 2	C.3
C.4	Fill Gas Composition History for PWR 15x15, Case 2	C.3
C.5	Fill Gas Composition History for PWR 17x17, Case 2	C.4
C.6	Gas Thermal Conductivity as a Function of Fill Gas Composition at 673K	C.4

TABLES

1	Fuel Rod Parameters for Comparison Study	12
2	Assumed Power Histories for Rod Type Comparison, Varying Peak Powers	14
3	Assumed Power Histories for Rod Type Comparison, 35 kW/m Peak Power	15
4	Assumed Input Uncertainties Common to All Rod Types	16
5	Gas Thermal Conductivity Uncertainty, Varying Peak Power	17
6	Gas Thermal Conductivity Uncertainty, 35 kW/m Peak Power	18
7	Uncertainty for Water Film and Cladding Temperatures at 35 kW/m	19
8	Elapsed Time and Burnup, Varying Peak Power	32
9	Elapsed Time and Burnup, 35 kW/m Peak Power	33
10	GT3 Predicted Relocation as a Function of Burnup	34
11	Basic Assumptions for BOL Uncertainty Parametric Study	41
12	Basic Assumptions for EOL Uncertainty Parametric Study	41
13	Assumptions of Parametric Plots of Minimum C_f Versus Resistance	69
14	Effect of Cracked Pellet Model on Relative Uncertainties	70

INTRODUCTION

During off-normal conditions in a nuclear reactor, the integrity of the fuel rods is highly dependent upon how high cladding temperatures become. These peak temperatures are dependent upon fuel rod conditions at the beginning of the off-normal period. To assess these initial conditions, vendors and regulators incorporate mathematical models into large computer codes; and to help assure appropriate use of these codes, the user must understand their accuracies and limitations.

In 1974, the Fuel Behavior Research Branch of the Nuclear Regulatory Commission (NRC) began a program to verify the accuracy of fuel performance computer codes and identify their limitations. This program, Experimental Support and Development of Single-Rod Fuel Codes,^(a) is being conducted at Pacific Northwest Laboratory (PNL).^(b) The program began with the irradiation of two fuel assemblies to extend the base of information regarding the behavior of reactor fuel during steady-state operation. This data base is being used to verify steady-state fuel performance computer codes (Hann et al. 1977). Since 1974 two more instrumented fuel assemblies have been included in the program. Steady-state and transient temperature data from these assemblies have been obtained and analyzed, ex-reactor testing to determine mechanical behavior of the fuel rod has begun, and error and uncertainty analysis has received increasing emphasis.

In 1977, program staff began estimating the uncertainty of thermal performance predictions that are based on steady-state fuel performance computer codes. This analysis utilized a technique called linear propagation of errors (LPE), which was found to be useful in predicting uncertainty. The work culminated with a report (Cunningham et al. 1978^(c)) that discussed how LPE could be applied to steady-state fuel codes and provided some results for a typical boiling water reactor (BWR) fuel rod.

(a) Prior to FY1980, this program was Experimental Verification of Steady-State Codes.

(b) Operated for the U.S. Department of Energy (DOE) by Battelle Memorial Institute.

(c) Hereafter, this report will be referred to as PNL-2581.

The work reported in PNL-2581 is expanded in this report in three main areas. First, this report compares the responses of BWR and pressurized water reactor (PWR) fuel rods during two postulated power histories. Second, a qualitative statement is presented discussing the processes of code verification and validation. Different approaches to answering the question of how the code relates to reality are presented. Finally, advancements in data analysis and fuel modeling over the last few years have shown that fuel cracking and relocation affect the thermal behavior of a fuel rod; therefore, this report includes a discussion on the effect of this concept change upon uncertainty analysis.

BACKGROUND

The work presented in this report relies heavily on the methodology developed and reported by Cunningham (PNL-2581). This section provides a summary of the LPE method, the ways it is applied, and sample results.

LINEAR PROPAGATION OF ERRORS

A common method used to predict the radial temperature profile of a fuel rod includes beginning with the coolant temperature and then, working radially inward, calculating the temperatures of different fuel rod regions.^(a) Thus, the calculations for a particular region, such as the gap between fuel and cladding,^(b) are dependent upon the calculations that preceded. This calculational scheme readily lends itself to estimating uncertainty by LPE. With this technique, estimated uncertainties are dependent upon input parameters and uncertainties and calculated variables and uncertainties. In addition, it is relatively easy to determine what percentage of an uncertainty estimate is due to a particular variable of interest.

LPE consists of first approximating the function of interest by a first-order Taylor's series and then approximating the variance of the function by the variance of the linear approximation. That is, if Y is a function of p variables

$$Y = F(X_1, X_2, \dots, X_p)$$

then it may be linearly approximated as

$$Y_L = F(\xi_1, \xi_2, \dots, \xi_p) + (X_1 - \xi_1) \frac{\partial F}{\partial X_1} + (X_2 - \xi_2) \frac{\partial F}{\partial X_2} + \dots + (X_p - \xi_p) \frac{\partial F}{\partial X_p}$$

(a) See Section 2 of PNL-2581

(b) Hereafter referred to as the fuel-cladding gap

where the X_i s are random variables that may or may not be interdependent and where

$$\frac{\partial F}{\partial X_i} = \frac{\partial F(X_1, X_2, \dots, X_p)}{\partial X_i}$$

is evaluated at $(X_1, X_2, \dots, X_p) = (\xi_1, \xi_2, \dots, \xi_p)$ where the ξ_i are the mean values or expected values of the X_i s.

Next, the absolute variance of Y is approximated by the absolute variance of the linear approximation

$$\sigma_Y^2 \approx \sigma_{Y_L}^2 = \sum_{i=1}^p \left(\frac{\partial F}{\partial X_i} \right)^2 \sigma_i^2 + 2 \sum_{i=1}^{p-1} \sum_{j>i} \left(\frac{\partial F}{\partial X_i} \right) \left(\frac{\partial F}{\partial X_j} \right) \sigma_{ij}$$

where σ_i^2 = the absolute variance of X_i

σ_{ij} = the covariance between X_i and X_j .

The validity of this approximation of the variance of Y depends on the following conditions:

- The variables X_i have finite means (μ_i) and variances (σ_i^2).
- The standard deviations of the X_i ($\sigma_i = \sqrt{\sigma_i^2}$) are small relative to their means (μ_i).

The latter is concerned with the adequacy of the approximation; that is, with how closely the summed linear terms of the Taylor's series expansion (Y_L) approximate the exact function Y over the range of variables in question. In terms of uncertainties, as defined in this report, the second requirement is that the X_i uncertainties be small.

The relative variance of $Y(C_Y^2)$ may now be defined as

$$C_Y^2 = \frac{\sigma_Y^2}{\mu_Y^2}$$

For intermediate variables that are interrelated, the relative covariance (C_{ij}) is found by

$$C_{ij} = \frac{\sigma_{ij}}{\mu_i \mu_j}$$

In this report, the percent uncertainty for a variable is determined from its relative variance by

$$\% U_Y = 300 \sqrt{C_Y^2}$$

This uncertainty estimate has a confidence level of 99.7%. In other words, assuming Y is normally distributed, Y will fall within the bounds of $\mu_Y \pm 3\sigma_Y$ 99.7% of the time. In this report, it is called a "3 σ confidence level."

Four conditions are important in obtaining meaningful results from the described method of linear propagation of uncertainty.

- For each input variable, the error (uncertainty) distribution is assumed Gaussian about a mean value. Moreover, the uncertainty is described adequately by the relative variance $C_i^2 = \sigma_i^2/\mu_i^2$. This implies that for the percent uncertainty to remain constant, the absolute variance must increase as the mean value increases.
- There is no covariance between any of the input variables; that is, there are no correlations between measurement errors for input variables.
- For the functions of interest the propagation of errors by first-order Taylor's series provides an adequate estimate of uncertainty.

- The uncertainty distributions for the derived variables (Y) are sufficiently symmetric for the first condition to be true.

The last of these conditions is related to determining the uncertainties for calculated values of thermal performance. If identical experiments could be run and parameters of interest could be measured under exact conditions, (burnup, time, power, etc.) for each experiment, a distribution of values for the variable could be obtained (this may be simulated by Monte Carlo techniques). Under this condition, such a distribution would be approximately symmetric about the mean value for the conditions of the experiment.

It is important to understand that LPE alone does not provide an estimate of bias between model and data; however, it does provide an estimate of the width of a normal distribution about the mean value of a calculated variable. To estimate bias, researchers must compare this predicted or modeled distribution with an observed distribution. (See Model and Code Verification section.)

APPLICATION OF LINEAR PROPAGATION OF ERRORS

This report includes a general uncertainty analysis of fuel rod temperatures and stored energy. A typical steady-state fuel performance code involves a complexity of models and iterative solutions that make application of LPE nearly impossible (see Figure 1). Therefore, the analysis was applied only to basic models. Since basic models are generally applicable to all fuel performance codes, LPE has in effect been applied to an abstract of fuel performance modeling. (Selected models are discussed in Appendix A.)

After the models of interest are chosen, the uncertainty equations are derived; these complex equations can be found in Appendix B of PNL-2581 and, therefore, are not repeated here. To facilitate the uncertainty analysis the models and uncertainty equations have been combined into the computer code STORE.

It should be recognized that although all codes may work from the same basic models, each code may use different material properties, have different secondary models, and apply different techniques for solution. Therefore,

FIGURE 1. Interrelationships of Variables and Models in a Fuel Performance Code

STORE is used in the following manner: First the code of choice--GAPCON-THERMAL-3 (GT3) (Lanning et al. 1978) in this report--is run on the problem of choice. Material properties, power history, and fuel rod changes (e.g., fission gas release, dimensional change, etc.) are used as input to STORE for the uncertainty analysis. Thus, the temperatures predicted by STORE match those of the code of choice, and the uncertainty predictions are applicable to the problem under study.

ASSIGNMENT OF UNCERTAINTY

Input parameters necessary for this analysis include design dimensions, material properties, and power. Assignment of uncertainties to these parameters is based principally on an examination of the measured variability of the input parameters. It can be difficult though to determine the confidence level of quoted uncertainties. For directly measured parameters where the measurements are provided (for example, fuel pellet diameter), the variance (σ_x^2) and confidence level are easily determined. However, when only an uncertainty is quoted (for example, power uncertainty is Z%), it then becomes necessary to assume the confidence level. In PNL-2581, it was generally assumed that quoted uncertainties were applicable at the 3σ confidence level.

In general, the input uncertainties used in PNL-2581 will hold for this report; the few changes are explained below.

Local Linear Heat Rate

Recently, there has been concern that the uncertainty level used in PNL-2581 was too low. The problem is that power uncertainties stated in the literature are often given without an attendant confidence level. An often found value of power uncertainty is 10%, and this value was used in PNL-2581 at a 3σ confidence level. However, the confidence level for the uncertainty estimate could range from 1σ (68.3%) to 3σ (99.7%). For this report, it has been concluded that the 10% value for power uncertainty should be applied with a 2σ confidence level rather than a 3σ confidence level. The corresponding 3σ confidence level power uncertainty is 15%.

Gas Thermal Conductivity

In PNL-2581, the uncertainty for gas thermal conductivity was based on the combined uncertainty of the gas mixture present in the fuel-cladding gap and the uncertainty in the prediction of the thermal conductivity for the assumed gas mixture. It was assumed that gas mixture uncertainty varied linearly from 0% at beginning-of-life (BOL) to 25% at end-of-life (EOL) while the model uncertainty varied from 2 to 6.5% for gases ranging from pure helium to typical fission gas mixtures; all of which resulted in a steadily increasing gas thermal conductivity uncertainty with burnup.

However, it may reasonably be assumed that at a certain point the gas composition will be nearly saturated with fission gas and the thermal conductivity uncertainty may be reduced. Therefore, a new method has been derived to assign gas thermal conductivity.

The primary question still remains: What is the gas composition uncertainty? The method now used is based on the following: First, the Beyer-Hann fission gas release model (Beyer and Hann 1974) is used in GT3 for temperatures greater than 1473K; for lower temperatures, the gas release model of Bellamy and Rich (1969) is used. Next, it was observed that for the GT3 runs being evaluated, predicted temperatures exceeded 1473K only at low burnup; therefore, the low-temperature gas release model was operative during the bulk of the GT3 modeling. Beyer and Hann assign an uncertainty of 1% to the low-temperature gas release model. This uncertainty is applied to the GT3 estimate of fission gas moles released, which produces upper and lower estimates of the amount of fission gas in the gap. Finally, the limits on gas composition are converted to thermal conductivities, and an uncertainty estimate is obtained by comparing the original thermal conductivity to the calculated limits. A minimum uncertainty of 2% is maintained. Appendix C provides further discussion and plots of fill gas composition as a function of burnup.

Fuel Thermal Conductivity

At BOL, the uncertainty for fuel thermal conductivity based on examination of data from unirradiated UO_2 is 10% (Hagman and Reymann 1979). During

irradiation, the effective thermal conductivity of the fuel matrix is expected to change because of fuel cracking and relocation. In addition, the entrapment of fission products within the UO_2 lattice may change the thermal conductivity of individual chunks of UO_2 . However, examination of burnup effects on the thermal conductivity of solid pieces of UO_2 reveals little effect above 1100K (Lokken and Courtright 1977). It is therefore concluded that the major effects on UO_2 thermal conductivity are caused by cracking and relocation. From analysis of in-reactor thermal data, it has been concluded that cracking and relocation are essentially concluded by 430 GJ/kgU (5000 MWd/MTM) of burnup. In addition, reductions of up to 20% have been deduced for the effective UO_2 thermal conductivity (Williford et al. 1980). Therefore, the uncertainty applied in this report for UO_2 thermal conductivity will vary linearly with burnup from 10% at BOL to 20% at 430 GJ/kgU; and 20% uncertainty will be assumed for all burnups greater than 430 GJ/kgU.

Flux Depression

During irradiation the flux depression within the fuel pellet primarily changes due to neutronics effects such as U-235 depletion and Pu build-in. Secondary causes of flux depression change might be physical effects such as fuel densification and relocation. Physical changes occur during the first 430 GJ/kgU of burnup while the neutronics changes occur over the lifetime of the fuel.

The flux depression uncertainty for this report will increase linearly from 5% at BOL (based on neutronics considerations) to 10% at 430 GJ/kgU. This may provide an initially high uncertainty number but should account for any effects throughout the postulated irradiation.

Specific Heat

Under steady-state conditions, specific heat affects the stored energy. From evaluation of data, the specific heat of UO_2 has an uncertainty of 5% at BOL (Kerrisk and Clifton 1972); for this report, it will increase linearly from 5% at BOL to 10% at 432 GJ/kgU to account for any factors that could change the specific heat.

SUMMARY OF PREVIOUS RESULTS

The work presented in PNL-2581 discussed the uncertainties in the predicted response of a BWR-6 fuel rod during startup and steady-state irradiation. The principal objectives of that work were to apply LPE to a steady-state fuel code, evaluate the applicability of LPE, and determine which code variables are most important to the uncertainties of predicted variables.

It was concluded that when compared to Monte Carlo evaluations, LPE is an adequate means to estimate uncertainty. Because LPE is applied to basic thermal models, the uncertainty predictions are generally applicable to steady-state fuel codes rather than being specific to only one code. Other conclusions that were reached include

- Good agreement was observed between the LPE uncertainty estimates for gap conductance and the observed variability of gap conductance as inferred from experimental data.
- Linear power, fuel thermal conductivity, and neutron flux depression (radial power profile) are the most influential parameters upon fuel centerline temperatures.
- The maximum uncertainties that occur are time dependent and generally increase with time.

FUEL ROD DESIGN ANALYSIS

The light water reactor (LWR) industry uses several basic fuel rod designs and operating conditions, which are modified as necessary from reactor to reactor. Designs can differ in dimension, fuel type, and power history. Because of these differences, questions arise as to their effects on thermal performance and uncertainty. This section presents an analysis of some standard designs and thereby a cursory and general evaluation of LWR fuel rod designs.

The selection of standard designs for an analysis of this type can be troublesome; however, four designs were specified during the assessment of FRAPCON-1 (Laats, Peeler, and Scofield 1979): BWR 7x7, BWR 8x8, PWR 15x15, and PWR 17x17. These and two additional designs were analyzed. BWR fuel rods are normally backfilled with helium at 1-atm pressure. Future BWR rods, however, may be backfilled at 3 atm to reduce the thermal effects of fission gas release; therefore, a BWR 8x8 rod with an initial pressure of 3 atm was included. PWR rods are normally backfilled with helium at 15-25 atm to counteract the high external pressure; for contrast, a PWR 17x17 rod at 1-atm pressure was included. Table 1 lists the fuel rod parameters used in this study.

TABLE 1. Fuel Rod Parameters for Comparison Study

Parameter	BWR 7x7	BWR 8x8	PWR 15x15	PWR 17x17
Cladding outer diameter, mm	14.30	12.52	10.77	9.50
Cladding inner diameter, mm	12.67	10.80	9.50	8.36
Fuel diameter, mm	12.37	10.57	9.31	8.19
Fuel enrichment, %	2.2	2.2	2.6	2.6
Fuel density, %TD	94	95	94	95
Plenum volume, cm ³	37.5	21.0	9.2	6.6
Fill gas pressure, MPa	0.10	0.10, 0.30	2.38	0.10, 2.03
Coolant pressure, MPa	7.14	7.27	15.51	15.51
Coolant temperature, K	551	551	561	561
Fuel/length, kg/m	1.239	0.914	0.702	0.549

This type of comparative examination must include power history. In an operating reactor, an LWR fuel rod will be exposed to a number of power cycles, several different sustained power levels, and shifts in core position. Thus, fuel rods from different reactors may have significantly different power histories. It would be impractical to try to duplicate this variety of power histories; however, since the general objective is to operate power reactors at constant power, the following assumptions were used to construct a useful power history:

- The rods are exposed to a constant neutron flux throughout the assumed irradiation exposure.
- Because of fuel depletion, each rod will experience decreasing power during the exposure.
- All rods are irradiated to a burnup of 2590 GJ/kgU (30 GWd/MTM).
- Two different initial rod peak powers are assumed: the core average for the rod design as stated in Table II of the assessment of FRAPCON-1 (Case 1) and 35 kW/m (Case 2).

Tables 2 and 3 summarize the assumed power histories.

As stated previously, the procedure for the uncertainty analysis is to first run the code of choice and then match STORE to the code results. The resulting uncertainty estimates from STORE may be considered applicable to the fuel performance code if appropriate input uncertainties are provided to STORE.^(a) Tables 4-6 list the assumed input uncertainties for the rod type analysis.

Table 7 lists predicted uncertainties for the water film temperature rise (ΔT_F), the cladding temperature rise (ΔT_C), and the cladding inner surface temperature (T_C). Several items are noteworthy.

(a) Assumes that the basic models in the code of choice are equivalent to those in STORE.

TABLE 2. Assumed Power Histories for Rod Type Comparison,
Varying Peak Powers

BWR 7x7		BWR 8x8		PWR 15x15		PWR 17x17	
BU ^(a)	PLHR ^(b)	BU	PLHR	BU	PLHR	BU	PLHR
0	0.0	0	0.0	0	0.0	0	0.0
0	6.6	0	6.6	0	6.6	0	6.6
0	13.1	0	13.1	0	13.1	0	13.1
0	19.7	0	19.7	0	19.7	0	19.7
1	26.3	1	26.3	1	26.3	1	25.0
2	34.0	1	29.0	1	32.0	4	25.0
13	34.0	3	29.0	4	32.0	22	25.0
26	34.0	15	29.0	21	32.0	44	25.0
53	34.0	31	29.0	43	32.0	89	25.0
107	33.9	62	29.0	88	32.0	177	24.8
187	33.7	124	28.9	175	31.8	266	24.7
266	33.6	216	28.7	263	31.7	353	24.6
346	33.4	308	28.6	350	31.6	441	24.5
425	33.3	399	28.4	437	31.5	528	24.4
503	33.1	490	28.3	524	31.3	615	24.3
581	33.0	581	28.1	610	31.2	702	24.3
659	32.8	671	28.0	696	31.1	788	24.2
737	32.7	760	27.8	782	31.0	874	24.1
814	32.5	849	27.7	867	30.8	959	23.9
891	32.4	938	27.6	952	30.7	1044	23.8
967	32.2	1026	27.4	1036	30.6	1129	23.7
1043	32.1	1114	27.3	1121	30.5	1213	23.6
1119	32.0	1201	27.1	1205	30.4	1297	23.5
1195	31.8	1288	27.0	1288	30.3	1381	23.4
1270	31.7	1375	26.8	1372	30.2	1464	23.3
1345	31.5	1460	26.7	1455	30.0	1547	23.2
1419	31.4	1546	26.6	1537	29.9	1629	23.1
1493	31.2	1631	26.4	1620	29.8	1712	23.1
1567	31.1	1716	26.3	1702	29.7	1794	23.0
1639	31.0	1800	26.2	1783	29.6	1875	22.9
1714	30.8	1883	26.0	1865	29.4	1957	22.8
1786	30.7	1967	25.9	1946	29.3	2038	22.7
1859	30.6	2050	25.8	2026	29.2	2118	22.6
1931	30.4	2132	25.6	2107	29.1	2198	22.5
2003	30.3	2214	25.5	2187	29.0	2278	22.4
2074	30.2	2296	25.4	2267	28.9	2358	22.3
2146	30.0	2377	25.2	2346	28.8	2437	22.2
2217	29.9	2459	25.1	2425	28.6	2516	22.1
2283	29.8	2538	25.0	2504	28.5	2595	22.0
2358	29.6			2583	28.4		

(a) BU = burnup in GJ/kgU

(b) PLHR = rod peak linear heat rate in kW/m

TABLE 3. Assumed Power Histories for Rod Type Comparison,
35 kW/m Peak Power

BWR 7x7		BWR 8x8		PWR 15x15		PWR 17x17	
BU (a)	PLHR (b)	BU	PLHR	BU	PLHR	BU	PLHR
0	0.0	0	0.0	0	0.0	0	0.0
0	6.6	0	6.6	0	6.6	0	6.6
0	13.1	0	13.1	0	13.1	0	13.1
0	19.7	0	19.7	0	19.7	0	19.7
1	26.3	1	26.3	1	26.3	1	26.3
1	31.2	1	32.8	1	32.8	2	32.8
2	35.0	3	35.0	4	35.0	5	35.0
13	35.0	18	35.0	23	35.0	30	35.0
27	35.0	37	35.0	47	35.0	61	35.0
55	35.0	74	35.0	96	34.9	123	34.9
110	34.8	149	34.8	192	34.8	247	34.7
192	34.7	260	34.6	287	34.7	370	34.5
274	34.5	371	34.4	383	34.5	450	34.3
356	34.4	481	34.2	478	34.4	615	34.1
437	34.2	590	33.9	572	34.2	736	33.9
518	34.1	698	33.7	666	34.1	856	33.7
598	33.9	806	33.5	760	33.9	975	33.5
678	33.8	913	33.3	853	33.8	1094	33.3
758	33.6	1020	33.1	946	33.6	1212	33.1
837	33.4	1126	32.9	1039	33.5	1330	32.9
916	33.3	1231	32.7	1131	33.3	1447	32.7
995	33.1	1335	32.5	1223	33.2	1563	32.6
1073	33.0	1439	32.3	1314	33.1	1678	32.4
1151	32.8	1542	32.1	1405	32.9	1793	32.2
1229	32.7	1645	31.9	1496	32.8	1907	32.0
1306	32.5	1747	31.7	1586	32.6	2021	31.8
1382	32.4	1848	31.5	1676	32.5	2133	31.6
1459	32.2	1949	31.3	1765	32.4	2246	31.4
1535	32.1	2049	31.1	1854	32.2	2357	31.2
1611	31.9	2149	30.9	1943	32.1	2468	31.0
1686	31.8	2247	30.7	2031	32.0	2578	30.9
1761	31.6	2346	30.5	2119	31.8		
1836	31.5	2443	30.3	2207	31.7		
1910	31.4	2540	30.2	2294	31.5		
1985	31.2			2381	31.4		
2058	31.1			2467	31.3		
2132	30.9			2553	31.1		
2205	30.8						
2277	30.6						
2350	30.5						
2422	30.4						
2493	30.2						
2565	30.1						

(a) BU = burnup in GJ/kgU

(b) PLHR = peak linear heat rate in kW/m

TABLE 4. Assumed Input Uncertainties Common to All Rod Types

	Uncertainty, %
Local linear heat rate (q)	15 ^(a)
Coolant temperature (T_W)	1
Fuel diameter (d_{fi})	0.2
Cladding inner diameter (d_{ci})	0.2
Cladding outer diameter (d_{co})	0.2
Fuel and cladding roughness (R)	10
Cladding thermal conductivity (K_C)	15
Fuel thermal conductivity (K_F)	(b)
Fuel specific heat (C_p)	(c)
Water film coefficient (h_f)	15
Contact conductance coefficients (C_2, C_3)	10
Temperature jump distance coefficient (a_g)	100
Fuel area function (F_p)	0.3
Fuel relocation parameter (F_{pr})	0.5
Flux depression (F)	(c)

(a) All uncertainties are for a 3σ confidence level.

(b) Varies linearly from 10% at 0 GJ/kgU to 20% at 432 GJ/kgU.

(c) Varies linearly from 5% at 0 GJ/kgU to 10% at 432 GJ/kgU.

TABLE 5. Gas Thermal Conductivity Uncertainty, Varying Peak Power (Case 1)

BWR 7x7		BWR 8x8			PWR 15x15		PWR 17x17	
BU ^(a)	UK _g ^(b)	BU	UK _g (1 atm)	UK _g (3 atm)	BU	UK _g	BU	UK _g
0	2.0							
0	2.0	0	2.0	2.0	0	2.0	0	2.0
0	2.0	0	2.0	2.0	0	2.0	0	2.0
0	2.0	0	2.0	2.0	0	2.0	0	2.0
1	2.0	0	2.0	2.0	1	2.0	1	2.0
2	2.0	1	2.0	2.0	1	2.0	1	2.0
13	2.0	1	2.0	2.0	1	2.0	4	2.0
26	2.0	3	2.0	2.0	4	2.0	22	2.0
53	2.0	15	2.0	2.0	21	2.0	44	2.0
107	3.4	31	2.0	2.0	43	2.0	89	2.0
187	6.2	62	2.3	2.0	88	2.0	177	2.0
266	9.3	124	3.5	2.0	175	2.0	266	2.0
346	12.7	216	7.7	2.8	263	2.0	353	2.0
425	16.3	308	11.1	4.2	350	2.0	441	2.0
503	20.4	399	14.8	5.7	437	2.0	528	2.0
581	24.7	490	18.5	7.3	524	2.0	615	2.3
659	28.0	581	22.2	8.9	610	2.0	702	2.7
737	29.4	671	26.4	10.7	696	2.2	788	3.2
814	30.2	760	30.7	12.5	782	2.6	874	3.7
891	30.6	849	35.0	14.3	867	3.0	959	4.2
967	30.7	938	39.8	16.3	952	3.4	1044	4.7
1043	30.8	1026	44.7	18.4	1036	3.8	1129	5.3
1119	30.4	1114	49.8	20.5	1121	4.3	1213	5.8
1195	30.0	1201	55.2	22.6	1205	4.8	1297	6.2
1270	29.4	1288	55.1	23.5	1288	5.0	1381	6.5
1345	28.8	1375	54.4	24.3	1372	5.4	1464	6.8
1419	28.1	1460	54.3	25.2	1455	5.6	1547	7.2
1493	27.3	1546	53.0	25.7	1537	5.9	1629	7.5
1567	26.5	1631	51.5	26.1	1620	6.2	1712	7.8
1639	25.6	1716	50.5	26.6	1702	6.4	1794	8.1
1714	24.9	1800	48.1	26.6	1783	6.7	1875	8.3
1786	23.8	1883	45.9	26.7	1865	6.9	1957	8.5
1859	22.7	1967	42.5	26.2	1946	7.1	2038	8.7
1931	21.5	2050	38.7	25.4	2026	7.3	2087	8.8
2003	19.9	2132	35.0	24.5	2107	7.4	2198	9.0
2074	18.3	2214	31.6	23.4	2187	7.6	2278	9.0
2146	16.8	2296	28.2	22.2	2267	7.6	2358	9.0
2217	15.3	2377	25.1	20.9	2345	7.7	2437	9.0
2283	13.9	2459	22.2	19.5	2425	7.7	2516	8.9
2358	12.6	2538	19.5	18.1	2504	7.7	2595	8.8
					2583	7.7		

(a) BU = burnup in GJ/kgU

(b) UK_g = gas thermal conductivity relative uncertainty, %

TABLE 6. Gas Thermal Conductivity Uncertainty, 35 kW/m Peak Power (Case 2)

BWR 7x7		BWR 8x8			PWR 15x15		PWR 17x17			
BU (a)	UK _g (b)	BU	UK _g (1 atm)	UK _g (3 atm)	BU	UK _g	BU	UK _g (20 atm)	BU	UK _g (1 atm)
0	2.0	0	2.0	2.0	0	2.0	0	2.0	0	2.0
0	2.0	0	2.0	2.0	0	2.0	0	2.0	0	2.0
0	2.0	0	2.0	2.0	0	2.0	0	2.0	0	2.0
0	2.0	0	2.0	2.0	1	2.0	1	2.0	1	2.0
1	2.0	1	2.0	2.0	1	2.0	1	2.0	1	2.0
1	2.0	1	2.0	2.0	1	2.0	2	2.0	2	2.0
2	2.0	3	2.0	2.0	4	2.0	5	2.0	3	2.0
13	2.0	18	2.0	2.0	23	2.0	30	2.0	10	2.0
27	2.0	37	2.0	2.0	47	2.0	61	2.0	16	2.0
55	2.0	74	2.8	2.0	96	2.0	123	2.0	28	2.0
110	3.4	149	5.2	2.0	192	2.0	247	2.0	41	2.0
192	6.4	260	9.4	3.4	287	2.0	370	2.0	59	2.3
274	9.6	371	13.7	5.2	383	2.0	450	2.0	91	3.8
356	13.1	481	18.1	7.1	478	2.0	615	2.3	122	5.2
437	17.0	590	22.8	9.1	572	2.0	736	2.9	184	8.5
518	21.2	698	27.7	11.2	666	2.1	856	3.6	276	13.0
598	25.6	806	32.9	13.4	760	2.5	975	4.3	369	17.7
678	28.4	913	38.4	15.7	853	2.9	1094	5.1	460	22.7
758	29.4	1020	44.2	18.1	946	3.4	1212	5.8	552	27.6
837	30.3	1126	50.5	20.7	1039	3.9	1330	6.3	643	32.8
916	30.7	1231	55.5	23.0	1131	4.4	1447	6.8	733	38.5
995	30.8	1335	54.7	23.9	1223	4.8	1563	7.2	824	44.4
1073	30.6	1439	54.0	24.8	1314	5.1	1678	7.7	914	50.8
1151	30.2	1542	52.9	25.6	1405	5.5	1793	8.1	1003	57.5
1229	29.7	1645	51.4	26.1	1496	5.8	1907	8.4	1092	64.5
1306	29.0	1747	49.8	26.6	1586	6.1	2021	8.7	1181	71.9
1382	28.4	1848	46.9	26.7	1676	6.3	2133	8.9	1269	72.7
1459	27.6	1949	43.2	26.3	1765	6.6	2246	9.0	1357	70.3
1535	26.9	2049	38.7	25.4	1854	6.9	2357	9.0	1444	67.6
1611	26.0	2149	34.3	24.3	1943	7.1	2468	8.9	1531	64.6
1686	25.2	2247	30.2	22.9	2031	7.3	2578	8.8	1618	61.5
1761	24.2	2346	26.3	21.4	2119	7.4			1704	59.2
1836	23.1	2443	22.7	19.8	2207	7.6			1790	55.5
1910	21.8	2540	19.4	18.1	2294	7.7			1876	51.5
1985	20.3				2381	7.7			1961	46.5
2063	18.7				2467	7.7			2046	41.3
2132	17.1				2553	7.7			2131	36.3
2205	15.6								2215	32.0
2277	14.1								2298	27.8
2350	12.8								2382	24.1
2422	11.5								2465	20.8
2493	10.3								2547	17.7
2565	9.2									

(a) BU = burnup in GJ/kgU

(b) UK_g = gas thermal conductivity relative uncertainty, %

TABLE 7. Uncertainty for Water Film and Cladding Temperatures at 35 kW/m

Rod Type	Relative Uncertainty, % (3σ)			Absolute Uncertainty, K $T_c \xi \pm 3\sigma$
	ΔT_F	ΔT_c	$T_c \xi$	
BWR 7x7	21.2	21.3	3.2	606 ± 19.1
BWR 8x8	21.2	21.3	3.7	617 ± 22.7
PWR 15x15	21.2	21.3	3.2	634 ± 20.0
PWR 17x17	21.2	21.3	3.2	636 ± 20.6

- For all rod types, the relative uncertainty for the cladding inner surface temperature is low (<4%).
- All rod types have the same relative uncertainty for the water film temperature rise because relative uncertainty depends only upon the sum of the variances of the parameters that are used to calculate the temperature rise and those parameters are assumed to be the same for all rod types.
- All rod types have the same relative uncertainty for the cladding temperature rise because the relative uncertainty depends principally on the uncertainty to the input parameters, rather than the value of the parameters.
- For both the water film and cladding temperature rises, the temperatures are power dependent; but their relative uncertainties are not. The relative uncertainty for the cladding inner surface temperature has a slight power dependency because the uncertainty equation includes the power-dependent temperatures.

The uncertainty of the cladding inner surface temperature will not receive further attention in this analysis because it is low--nearly constant between rod types--and unchanging with burnup.

Figures 2-12^(a) visually summarize the rod type analysis. Each figure includes as a function of burnup^(b) the GT3 predictions of fuel surface temperature, fuel centerline temperature, and stored energy above coolant,^(c) along with the absolute uncertainty bounds^(d) (3σ confidence level) as predicted by STORE. These figures illustrate the effect of design differences; from them, certain deductions can be made.

FUEL ROD TEMPERATURES

Beginning with the predicted thermal response of the fuel rod designs, there is a difference between the peak centerline temperatures of the different fuel rod designs at BOL. At 35 kW/m, those temperatures are

BWR 7x7	1746K
BWR 8x8 (1 atm)	1696K
BWR 8x8 (3 atm)	1681K
PWR 15x15	1661K
PWR 17x17	1654K

The differences in peak temperature are directly associated with the initial gap size. The BWR 7x7 has the largest gap and the highest temperature, and the PWR 17x17 has the smallest gap and the lowest temperature. The 3-atm BWR 8x8 rod has a slightly lower temperature than the 1-atm rod because the extra helium provides some improvement in gap conductance.

The most obvious feature of Figures 2-12 is the rapid drop in temperature early in life. This drop is due to the relocation model in GT3 that specifies the change in the radial gap (Δd_g) as a function of power (q) and burnup (BU):

-
- (a) These figures begin with the first full power step after the rise to power.
 (b) Tables 8 and 9 relate the burnup in the figures to elapsed time of irradiation for each rod design.
 (c) For each rod type, the stored energy between 293K and coolant temperature is: BWR 7x7 = 8.67×10^4 J/m, BWR 8x8 = 6.39×10^4 J/m, PWR 15x15 = 5.44×10^4 J/m, PWR 17x17 = 4.21×10^4 J/m. The conversion for J/m to BTU/lbm for each rod type is: BWR 7x7 = 0.3466, BWR 8x8 = 0.4698, PWR 15x15 = 0.6117, PWR 17x17 = 0.7821.
 (d) These bounds are indicated on the figures by arrowheads.

FIGURE 2. Thermal History for BWR 7x7, 34 kW/m Peak Power

FIGURE 3. Thermal History for BWR 8x8, 29 kW/m Peak Power

FIGURE 4. Thermal History for BWR 8x8, 3 atm, 29 kW/m Peak Power

FIGURE 5. Thermal History for PWR 15x15, 32 kW/m Peak Power

FIGURE 6. Thermal History for PWR 17x17, 25 kW/m Peak Power

FIGURE 7. Thermal History for BWR 7x7, 35 kW/m Peak Power

FIGURE 8. Thermal History for BWR 8x8, 35 kW/m Peak Power

FIGURE 9. Thermal History for BWR 8x8, 3 atm, 35 kW/m Peak Power

FIGURE 10. Thermal History for PWR 15x15, 35 kW/m Peak Power

FIGURE 11. Thermal History for PWR 17x17, 35 kW/m Peak Power

FIGURE 12. Thermal History for PWR 17x17, 1 atm, 35 kW/m Peak Power

TABLE B. Elapsed Time and Burnup, Varying Peak Power

BWR 7x7		BWR 8x8		PWR 15x15		PWR 17x17	
TIME ^(a)	BU ^(b)	TIME	BU	TIME	BU	TIME	BU
1	2	1	3	1	4	1	4
5	13	5	15	5	21	5	22
10	26	10	31	10	43	10	44
20	53	20	62	20	88	20	89
40	107	40	124	40	175	40	177
70	187	70	216	60	263	60	266
100	266	100	308	80	350	80	353
130	346	130	399	100	437	100	441
160	425	160	490	120	524	120	528
190	503	190	581	140	610	140	615
220	581	220	671	160	696	160	702
250	659	250	760	180	782	180	788
280	737	280	849	200	867	200	874
310	814	310	938	220	952	220	959
340	891	340	1026	240	1036	240	1044
370	967	370	1114	260	1121	260	1129
400	1043	400	1201	280	1205	280	1213
430	1119	430	1288	300	1288	300	1297
460	1195	460	1375	320	1372	320	1381
490	1270	490	1460	340	1455	340	1464
520	1345	520	1546	360	1537	360	1547
550	1419	550	1631	380	1620	380	1629
580	1493	580	1716	400	1702	400	1712
610	1567	610	1800	420	1783	420	1794
640	1639	640	1883	440	1865	440	1875
670	1714	670	1967	460	1946	460	1957
700	1786	700	2050	480	2026	480	2038
730	1859	730	2132	500	2107	500	2087
760	1931	760	2214	520	2187	520	2198
790	2003	790	2296	540	2267	540	2278
820	2074	820	2377	560	2345	560	2358
850	2146	850	2459	580	2425	580	2437
880	2217	880	2538	600	2504	600	2516
910	2283			620	2583	620	2595
940	2358						

(a) TIME = elapsed time in days

(b) BU = burnup in GJ/kgU

TABLE 9. Elapsed Time and Burnup, 35 kW/m Peak Power

BWR 7x7		BWR 8x8		PWR 15x15		PWR 17x17	
TIME ^(a)	BU ^(b)	TIME	BU	TIME	BU	TIME	BU
1	2	1	3	1	4	1	5
5	13	5	18	5	23	5	30
10	27	10	37	10	47	10	61
20	55	20	74	20	96	20	123
40	110	40	149	40	192	40	247
70	192	70	260	60	287	60	371
100	274	100	371	80	383	80	493
130	356	130	481	100	478	100	615
160	437	160	590	120	572	120	736
190	518	190	698	140	666	140	856
220	598	220	806	160	760	160	975
250	678	250	913	180	853	180	1094
280	758	280	1020	200	946	200	1212
310	837	310	1126	220	1039	220	1330
340	916	340	1231	240	1131	240	1447
370	995	370	1335	260	1223	260	1563
400	1073	400	1439	280	1314	280	1678
430	1151	430	1542	300	1405	300	1793
460	1229	460	1645	320	1496	320	1907
490	1306	490	1747	340	1586	340	2021
520	1382	520	1848	360	1676	360	2133
550	1459	550	1949	380	1765	380	2246
580	1535	580	2049	400	1854	400	2357
610	1611	610	2149	420	1943	420	2468
640	1686	640	2247	440	2031	440	2578
670	1761	670	2346	460	2119		
700	1836	700	2443	480	2207		
730	1910	730	2540	500	2294		
760	1985			520	2381		
790	2063			540	2467		
820	2132			560	2553		
850	2205						
880	2277						
910	2350						
940	2422						
970	2493						
1000	2565						

(a) TIME = elapsed time in days

(b) BU = burnup in GJ/kgU

where $B = \exp(-4 + BU^{1/4})$ and GAP is the initial (cold) diametral gap. It can be seen that once full power is reached^(a) this relationship is dependent only on burnup and, as shown in Table 10, reaches a maximum value after a burnup of 400 GJ/kgU. This value corresponds to the time in the irradiation when the rapid temperature drop is completed.

After 400 GJ/kgU, the temperature behavior is dependent upon the slowly decreasing linear heat rate (which will drop temperatures) and the increasing amount of fission gas present in the fuel-cladding gap (which will raise temperatures). At this point, fuel rod design begins to show a significant effect.

Although Figures 2-12 present the predicted fuel centerline and surface temperatures as a function of burnup, there is a better indicator of the

TABLE 10. GT3 Predicted Relocation as a Function of Burnup

Burnup, GJ/kgU (MWd/MTM)	$\frac{B}{1+B}$	Δd_g , mm (in.)
0 (0)	0.01779	0.01524 (0.00060)
9 (100)	0.30201	0.02896 (0.00114)
43 (500)	0.67452	0.04674 (0.00184)
86 (1000)	0.83527	0.05461 (0.00215)
130 (1500)	0.90233	0.05766 (0.00227)
173 (2000)	0.93628	0.05944 (0.00234)
259 (3000)	0.96773	0.06096 (0.00240)
346 (4000)	0.98116	0.06147 (0.00242)
432 (5000)	0.98798	0.06172 (0.00243)

$$B = \exp(-4 + BU^{1/4}), \text{ BU in MWd/MTM}$$

$$\text{GAP} = 0.230 \text{ mm (0.009 in.)}, \text{ diametral}$$

$$q = 35 \text{ kW/m (10.67 kW/ft)}$$

(a) The model as written assumes that once the fuel has relocated toward the cladding it cannot retreat; therefore, should the power drop, fuel relocation would not be reduced.

changes within a fuel rod. Figures 13 and 14 present the thermal resistance^(a) of the fuel rods as a function of burnup. Appendix B provides a more detailed discussion of the resistance concept.

The BOL drop in fuel centerline and surface temperatures seen in Figures 2-12 is also observed in Figures 13 and 14; however, after this temperature drop differences between the rod designs are observed. The BWR centerline temperatures in Figures 2-4 and 7-9 appear fairly constant with only a slight increase at EOL. However, the resistance for the 1-atm BWR rods begins increasing immediately after the fuel relocation is completed. This increase in resistance is directly attributable to the release of fission gas to the fuel-cladding gap, which degrades the gap conductance.

This emphasizes the importance of increasing the initial amount of helium in a fuel rod. Notice the resistance for the 3-atm BWR rod: Initially it is constant (after relocation is completed) and does not begin to rise until later in life. This is because fission gas release cannot degrade the thermal conductivity of the fill gas as quickly and thus reduce the gap conductance.

The PWR centerline temperatures in Figures 5, 6, 10, and 11 are seen to decrease with burnup. Figures 13 and 14 show that the resistance for these rods remains constant during the assumed power history. Therefore, the observed temperature drop is directly attributable to the power decrease during the power history. The constant resistance indicates that fission gas release has a negligible effect on the gap conductance. As with the 1-atm BWR rods, resistance for the 1-atm PWR rod begins increasing after relocation is complete (Figure 14). At EOL, its resistance is 30% higher than that of the pressurized PWR rods.

Figure 14 indicates that for approximately equal power and after relocation has been assumed, the 7x7 BWR rod has a lower resistance than the 8x8 BWR rod and the 15x15 PWR rod has a lower resistance than the 17x17 PWR rod. It was noted earlier that at BOL increasing gap sizes lead to higher fuel temperatures, which is the opposite of the effect here. After relocation each rod

(a) The thermal resistance is defined as the difference between the fuel centerline temperature and coolant temperature divided by the local linear heat rate.

FIGURE 13. Thermal Resistance History for Case 1

FIGURE 14. Thermal Resistance History for Case 2

type has approximately the same gap conductance and fuel surface temperature, which would seem to lead to equal resistances. However, to produce the same linear heat rod, the smaller diameter rod must have a higher power density. This then results in a higher centerline temperature and the observed higher resistance for the smaller diameter fuel rods.

TEMPERATURE UNCERTAINTY

Figures 2-12 present the estimated uncertainty for temperature and stored energy as upper and lower bounds. Several general observations can be made from these plots.

- The uncertainty for fuel surface temperature decreases when fuel-cladding contact occurs because it is assumed that gap conductance is better defined under contact conditions.
- The width of the uncertainty band for fuel surface temperature increases with burnup because of an increasing contribution from the fuel relocation factor (F_{pr}).
- Although the fuel surface temperature uncertainty decreases under fuel-cladding contact conditions, the uncertainty of centerline temperature and stored energy does not decrease at this point. This occurs because power is the principal driver of fuel temperatures and is therefore the major contributor to and dominator of fuel uncertainties. If the assigned power uncertainty was less than 15% (3σ), a decrease in fuel centerline temperature and stored energy uncertainty would be seen when the fuel surface temperature uncertainty decreases. This result is also seen with Monte Carlo analysis.

While the temperature and absolute uncertainty response differs from rod to rod, the relative uncertainty (expressed as a percent of the predicted parameter) is nearly equal between rod designs. This particularly holds true at BOL before burnup effects make substantial changes to the operating conditions. Therefore, parametric plots have been developed that present the relative uncertainty for centerline temperature and stored energy as a function of power uncertainty.

Figures 15-17 present BOL relative uncertainty plots for power levels of 20, 35, and 50 kW/m; and Table 11 lists basic assumptions. Three assumptions for fuel thermal conductivity, specific heat, and flux depression uncertainty are used to provide a band of relative uncertainty. It can be noted that

- Uncertainties for fuel centerline temperature and stored energy are nearly linear with power uncertainty when power uncertainty exceeds 20%.
- Uncertainties for fuel thermal properties and radial power distribution define the minimum uncertainty for temperature, stored energy, and the width of the uncertainty band as a function of power.

Table 12 presents the uncertainties used for developing parametric plots for EOL conditions. Because of the difference in time-dependent response between BWR and PWR designs, a single plot cannot be developed for both designs. Results for a BWR rod are shown in Figures 18-20 and results for a PWR rod are shown in Figures 21-23. The same general trends observed in the BOL figures can be seen with the major exception being the lower values of relative uncertainty (relative uncertainty is inversely proportional to temperature). Although the higher EOL temperatures have a lower relative uncertainty, the absolute uncertainty (in K for temperature or J/m for stored energy) is larger than at BOL because of the higher temperatures at EOL.

The uncertainty estimates provided in this section serve a dual purpose. First, as presented, they provide confidence bands for modeling predictions of fuel rod thermal behavior; i.e., a prediction of X is good within $\pm Y\%$. Secondly, because the models are predicting behavior, it would be expected that observed data would fall within the band described by the uncertainty analysis if the modeling is done correctly. This leads into the next subject: verification and validation of models and computer implementations of those models.

FIGURE 15. Beginning-of-Life Relative Uncertainty for a LWR Rod at 20 kW/m

FIGURE 16. Beginning-of-Life Relative Uncertainty for a LWR Rod at 35 kW/m

FIGURE 17. Beginning-of-Life Relative Uncertainty for an LWR Rod at 50 kW/m

FIGURE 18. Beginning-of-Life Relative Uncertainty for an LWR Rod at 35 kW/m

TABLE 11. Basic Assumptions for BOL Uncertainty Parametric Study

THERMAL RESPONSE						
Power, kW/m	Resistance, (a)		Centerline		Stored Energy, (b)	
	mK/W · 100		Temperature, K		J/m	
	BWR	PWR	BWR	PWR	BWR	PWR
20	2.6	2.6	1073	1096	94,400	55,900
35	2.6	2.6	1463	1479	154,900	90,500
50	2.9	2.9	1980	2021	240,600	145,200

INPUT UNCERTAINTY

Parameter	Curve (% Relative Uncertainty, 3σ)		
	A	B	C
Fuel Thermal Conductivity	10	20	30
Fuel Specific Heat	5	10	15
Flux Depression	5	10	15
Gas Thermal conductivity	5	5	5

(a) Resistance based on GT3 predictions with fuel relocation.
Higher resistance at 50 kW/m is due to reduced fuel thermal conductivity at higher temperatures.

(b) Stored energy is relative to coolant temperature.

TABLE 12. Basic Assumptions for EOL Uncertainty Parametric Study

THERMAL RESPONSE						
Power, kW/m	Resistance, (a) mK/W · 100		Centerline Temperature, K		Stored Energy, (b) J/m	
	BWR	PWR	BWR	PWR	BWR	PWR
	20	4.2	3.1	1393	1198	179,600
35	3.9	3.0	1917	1629	270,100	112,000
50	3.7	2.9	2393	2052	349,300	149,500

INPUT UNCERTAINTY

Parameter	Curve (% Relative Uncertainty, 3σ)		
	A	B	C
Fuel Thermal Conductivity	10	20	30
Fuel Specific Heat	5	10	15
Flux Depression	5	10	15
Gas Thermal conductivity	15	15	15

(a) Because of fission gas release, resistance is gap dominated.

(b) Stored energy is relative to coolant temperature.

FIGURE 18. End-of-Life Relative Uncertainty for a BWR Rod at 20 kW/m

FIGURE 19. End-of-Life Relative Uncertainty for a BWR Rod at 35 kW/m

FIGURE 20. End-of-Life Relative Uncertainty for a BWR Rod at 50 kW/m

FIGURE 21. End-of-Life Relative Uncertainty for a PWR Rod at 20 kW/m

FIGURE 22. End-of-Life Relative Uncertainty for a PWR Rod at 35 kW/m

FIGURE 23. End-of-Life Relative Uncertainty for a PWR Rod at 50 kW/m

MODEL AND CODE VERIFICATION

The end objective of developing fuel rod behavior models is to be able to predict how fuel rods will behave. Once the desired models have been selected/developed, implemented as a computer code, and a prediction obtained, the question arises: How good is the prediction? Points to be considered when answering this question include accuracy of the chosen models, quality of the input to the computer code, and, in general, confidence in the code.

This section presents a qualitative discussion of the modeling process and code validation. Examples of several techniques that have been used to support the validity of computer codes have been included.

MODELING AND REALITY

The process of model development is usually not discussed when model validation is the main interest; however, this process is a factor in assessing the confidence to be given to a model. It also provides a common ground from which the terms model verification, validation, and evaluation may be later defined.

Mar (1974) in discussing the process of structuring models states that the development follows a general pattern of explicit mental models, correlative models, and casual models. First, a model is constructed based on experience, intuition, and limited data to provide quantitative insights. Second, as additional quantitative data become available, a model is developed based on those data and empirical correlation of significant parameters. Third, physical theories plus quantitative data are employed to develop a model. In the physical sciences, theories and data are usually available to develop basic models that are generally accepted. However, even in well-developed physical science areas (for example, nuclear fuel thermal and mechanical performance) detailed theory and extensive data may not always be available to describe a model completely. Some components of a model will therefore be based on empirical correlations and others only on intuition, experience, and limited data. Recognition of these stages or steps in model development is important when confidence in a model is assessed.

The basic components inherent in the modeling process are the true physical situation, the observed physical situation, accepted scientific knowledge, and the resulting theoretical model. The relationship among these components is shown in Figure 24. It is the objective of the modeler to develop a theoretical model that adequately depicts the true physical situation. The theoretical model is based on accepted scientific knowledge and the observed or perceived physical situation.

The actual physical situation may be described as the true state of nature. For nuclear fuel performance this includes the actual state of the fuel, cladding, fill gas, coolant, and many additional factors associated with nuclear reactor operation. The factors may be classified roughly into initial conditions, controllable operating conditions, and resulting operating conditions or states. Initial conditions are typified by fuel, cladding, and general reactor characteristics. Controllable operating characteristics are power level and coolant conditions. Operating characteristics are those that are determined by initial conditions and controllable operating characteristics. These include fuel radial temperature profile, cladding temperature, fission gas composition, and fuel-cladding mechanical behavior as well as many others.

The process of observing or perceiving the true physical situation induces noise or error in the resultant observations or perceptions. This arises from the process of measuring a certain characteristic or when perceptions are filtered by previous knowledge. In many cases the error introduced is inconsequential to the development of the theoretical model; in others it may actually lead to an incorrect model or at least an incorrect empirical parametric formulation. For example, if a thermocouple is placed in the center of the fuel to measure the fuel centerline temperature, it may actually change the physical

FIGURE 24. Components of Modeling Process

situation: Since part of the fuel is removed to accomplish the measurement, the centerline temperature is changed. Although adjustments in the measured centerline temperature can be made, it is the resulting adjusted temperature that enters into the development of the theoretical model.

An advantage of developing a theoretical model in the physical sciences is the rich history of theory and related data available; hence, much of the model development is based on accepted scientific knowledge. However, the use of scientific knowledge in model development is not always done without the introduction of noise (error). For example, in constructing a theoretical model to describe fuel rod behavior, it is often necessary to approximate or simplify certain aspects of accepted scientific knowledge (represented in Figure 24 as the introduction of noise between components). In GT3 the radial temperature profiles can be theoretically described by a coupled set of equations in three dimensions. In actual application the equations are simplified to include only the radial direction. This approximation, and the numerical algorithm used for its solution, introduces noise (for lack of a better term) to the information.

The observed or perceived physical situation is also a part of the development of a theoretical model. In many cases there is no accepted theory; only empirical information is available for formulating possible mechanisms. Much of this information is gained from observing and analyzing previous experiments. In some cases a theoretical mechanism can be formulated but an empirically determined parametric function must be used to implement the mechanism as part of a working model. In this case the theoretical model is based on actual physical situations, but approximation and/or noise is introduced by the process of observing the actual situation and by simplifying the observed situation by means of a mathematical formulation.

A distinction is made between the theoretical model, which includes the mathematical formulation and supporting empirical parameterizations, and the implementation of the theoretical model as a computer code or model. Confidence in the computer model is enhanced by increased understanding of the basis for the theoretical model. This understanding may be increased by providing

in separate documentation a detailed description of the philosophy used in developing the model, the reasoning behind the selection of the approach, and the components of the model.

It is necessary to emphasize that documenting the development process for a theoretical model is an important part in the subsequent assessment of the model as a computer code. The documentation of the process, including the model selected and the reasons for the choice, is the mechanism for informing users. The documentation must give a clear definition of the system modeled and its proposed use plus a clear understanding of the status of theory, experience, intuition, and data for each component in the system. This does not imply that each component of the model must be state of the art, only that its relationship to the state of the art be given.

A computer code is the implementation of a theoretical model, and it is a distinct step in the modeling process and should not be combined with the development of the theoretical model. It is recognized that interactions occur between the steps and iterations do occur in the process. The construction of the computer code is not a direct translation from a detailed theoretical model.

Implementation of the theoretical model usually requires iterative solutions and/or numerical approximations. For example, in GT3 and the FRAPCON code series, the theoretical model for radial temperature profile is solved by using the technique of orthogonal collocation of weighted residuals. To develop confidence in these codes, it is not only necessary that the theoretical model be accepted but also the choice of the numerical technique. Documentation supporting the technique in the present application is necessary for developing confidence in the model.

Computer code implementation may involve additional approximations or assumptions. As previously indicated, numerical approximations are usually required to implement the theoretical model. Their use introduces noise between the computer code implementation and the theoretical model. The implementation introduces coding errors or inadequacies. Hopefully, these can be easily eliminated. The finite accuracy of the computer can also introduce

noise in implementing the theoretical model. All of these factors must be considered.

The theoretical model and its computer code implementation can be distinguished by the code's dependence on a particular computer operating system; the theoretical model is independent of computers. Thus, the model must stand alone and be evaluated accordingly. Justification and documentation of the model must be sufficient to allow an independent assessment of its merits. This is especially critical when the model is to be used in situations where it is impossible to check model predictions against actual observed data. The computer code cannot be assessed independently of its computing system environment; therefore, a change in the computing system requires a reevaluation of and occasionally a redesign of the code even though the theoretical model has not changed.

CODE VERIFICATION

Code verification is defined as the process of verifying that the computer code implementation of the model is done correctly. Commonly, code verification is assumed to be the same as debugging a computer code; however, debugging is only a part of code verification. When numerical approximations have been used, the solution accuracy needs to be evaluated and checked for the possibility of multiple solutions. The stability of algorithms must be investigated, especially for models predicting a time history. Theoretically an algorithm may be known to be stable but the finite accuracy of the computer may invalidate the stability.

Code verification encompasses only the theoretical model, the code implementation, past observed physical situations used to develop the model, and elements of accepted scientific knowledge (Figure 25). The only concern is: Does the computer code in the present computing environment accurately represent the theoretical model? At this stage it is not of concern whether the computer code agrees with the actual or observed physical situation.

In addition to careful documentation of the design and implementation of the computer code and comparison of code predictions with analytical results

FIGURE 25. Computer Code Implementation of Theoretical Model

where possible, active debugging is important. Active debugging concerns the process of running the code to find hidden errors, which is not a trivial task for complex codes such as GT3. The number of input variables, their allowable ranges, and the number of options quickly result in a large number of combinations to be checked in separate computer runs. Statistical concepts of experimental design can be used to reduce the number of computer runs required. One application of this concept is given by McKay, Conover, and Beckman (1979), although in a different context.

Except with relatively simple models, a computer code is rarely completely verified. Verification is limited by the knowledge available about what the theoretical model implies in specific cases. This is especially true concerning magnitudes of output variables. Generally, the only comparison available is whether the result "looks reasonable." Another limitation is the inability to try all possible combinations. Stated in a statistical context, an inference is required in stating that a computer code is verified. The strength of or confidence placed in this inference depends on all aspects of model verification and not just selected computer results.

MODEL ANALYSIS

Model analysis is concerned with gaining an understanding of the theoretical model. The importance of selected variables or the change in an output

variable as a function of changes in input variables may be investigated. Although model analysis can be completed on the theoretical model directly, it is usually conducted by using the computer code implementation in a sensitivity study. In general, the emphasis is on gaining an understanding of the relationship between output and input variables; and in some cases the contribution of complete submodels is investigated.

Model analysis can contribute to the development of confidence in a theoretical model through an increased understanding of the inner workings of the model. Secondary consequences of a theoretical model may also be checked through model analysis to further increase confidence in the model. However, model analysis as defined here will not directly support the correctness of the theoretical model in representing the actual physical situation.

MODEL VALIDATION

Model validation may mean many things. For present purposes a relatively restricted definition is given. Model validation is the comparison of output from a computer code implementation of a theoretical model to data obtained from an observed physical situation. Preferably the observed data are the product of a planned experiment so that the conditions under which the data are collected are well controlled and measured.

The term model validation has been criticized by many authors. Mitchell and Wilson (1979) have given some of the main reservations:

- It implies that it is possible to establish the validity of a model.
- It ignores the role of the use of the model.
- It ignores the temporary nature of model "validity."
- It ignores the role of subjectivity in the validation process.

Although these reservations apply to a more general definition of model validation than presently assumed, they do highlight important points both in model validation and in developing confidence in a model. In fact, the concept of developing confidence in a model coincides with some authors' definition of model validation.

Since the use of the model must be considered as an integral part of model validation, it is generally not possible to validate a model for all possible

uses. Therefore, the first step in model validation must be a clear definition of the use for which the model is being validated.

Model validation, as applied in the usual way, has a sense of concreteness associated with it. The association of the validation with an end use erodes that idea of finality or definiteness, and it is further eroded when the subjective and temporary nature of the validation is accepted. Validation is subjective since the physical situation is observed with error, which affects not only the comparison of the output with observed data but also the selection of input values for the code.

After clearly stating the end use, the next step is to determine how precisely and accurately the identified variables must be predicted for the model to be considered useful. This viewpoint stresses a yes/no decision on model validity for a particular use, and it presumes that it is possible to obtain observed data to make the necessary comparisons. If adequate data cannot be obtained, a formal determination of the validity of the model for that use cannot be made.

The term model validation implies that it is possible to establish the validity of the model. If a model has not yet been validated, the implication is that if more effort were expended (i.e., more experimental data gathered and compared to model output) it would only be a matter of time before the model would be validated. This implication ignores the dependence on the end use of the model and the known introduction of noise between the theoretical model, the true physical situation, and accepted scientific knowledge. The useful question is: Does the computer code implementation agree closely enough with the physical situation for a specific use? Segments of the model may be known to be invalid (incorrect or only approximations); but if the model output is satisfactory for the end use, the model remains useful. As a result the model may be inadequate for another use.

Conceptually, the process of model validation is simple. An end use of the model is described and criteria are selected for determining if the model is adequate enough for the use. An experiment is planned and executed or previously gathered data are found that meet the requirements for the

validation exercise. Values for the input variables are chosen to match the experimental conditions and the computer model is executed. The model output is then compared to corresponding observed experimental data. In practice, however, there are many difficulties that may arise.

Since most models produce a time history on a number of variables, a large number of individual comparisons are definable. The comparisons that are to be included in the validation must be described clearly, for it is probable that not all of them will indicate that the model is valid. A subjective assessment, or in rare cases a quantitative measure, must be made concerning overall model validity. It is easy to envision a large number of comparisons for even a single physical situation.

In practice, determining the validity of a model for even a single end use will require that a number of physical situations be included in the validation process. Clearly, obtaining observed data will not be feasible for all situations; and, therefore, some representative cases must be selected. In the physical sciences the continuity or smoothness of most physical processes is a distinct advantage. The end use of the model naturally leads to a definition of ranges appropriate for each of the input variables to the model. More generally this is termed the feasible region for the input variables for that end use. By using the basic concepts of experimental design, a series of experiments may be defined that will allow an inference to be made on the validity of the model. This is a luxury that is available only if it is possible to conduct experiments with input variables in the feasible region. The concept of designed experiments can be profitably used in model verification where observations of the physical situation are not needed.

More commonly a few previously conducted experiments and additional observations are available from normal operations and routine measurements. Rarely do these experiments and observations result in data covering the feasible region of input variables, and only occasionally are they near the feasible region. Clearly the formal validation process is curtailed or even invalidated in that particular case and must be replaced in this situation by a face validation. Face validation, which is much weaker than formal validation, is

based on comparisons made outside the feasible region, if any; confidence in the model is developed through model verification, analysis, and documentation.

Given the input values to the code, the output is fixed and may differ from the observed data due to

- observation error in the data
- input to the code that differs from the true physical situation
- an inadequate model.

Any or all of these can be present in a model validation exercise, and it is difficult to determine if there is an inadequacy in the model that affects the usefulness of the model when other causes for discrepancy are possible.

In most validation studies it is assumed that input variables (initial conditions) are known without error. All differences between model output and observed data are attributed either to model inadequacies or experimental error in the observed output variables. Typically in the physical sciences it is possible to estimate (guesstimate?) the error in the observed variables. The predicted output is compared to the observed data with its associated error limits. If the prediction is within the error limits, it is inferred that the model is adequate; if not, model adequacy is questioned. This procedure depends heavily on the correct assessment of the error associated with the observed data. Hence, model validation depends on an error analysis of the observed data or physical situation; when errors in input variables are admitted, the comparison becomes even more subjective.

An alternative approach to model validation is available that assumes that there are errors in input and output variables. Conceptually the idea is to adjust the model input variables so that model output agrees exactly with observed output data. The model validation comparison is then between observed input values and empirically determined model input values. The model is validated when the input values do not differ significantly. The process, however, is complicated by having to determine model input values; and a trial-and-error approach can be expensive. A further complication is the

possibility that more than one choice of model input values can lead to the same model output values. Knowledge of such multiplicity can be very enlightening however.

The preceding comments certainly do not cover all the topics connected with developing confidence in a model nor are those included discussed in any depth. However, those individuals looking for a well-defined procedure that will lead to the validation of a model for all applications for which it was designed will be disappointed; those looking for specific statistical techniques to use have not been satisfied. These comments are not what model developers want to hear.

Briefly, the position taken is that while it is not possible to validate a model in the usual sense, it is possible to develop confidence in a model. The level of confidence will depend upon who is studying the model and will change with time. Model developers and users must make a distinction between face validity and formal validity. Formal validity is only possible when observed data for a feasible region of input variables are available for comparison with model output predictions; face validity depends only on model documentation, verification, and analysis and is therefore weaker. This does not imply that gaining face validity for a model is an easy task; in a sense, it is more difficult since it rests solely on communication of model characteristics and defense of the correctness of the logic behind the model.

EXAMPLES OF VALIDATION

Having discussed the process and problems of validating theoretical models, it is useful to present several examples of model validation.

The first example is the code verification and model validation of GT3 (Lanning, Panisko, and Mohr 1978). The work was divided into three basic areas

- Mathematical consistency of the coding was verified by comparison to hand calculations and analytical solutions. Simplifications in the code, such as elimination of temperature-dependent properties, were often necessary for this comparison. Figure 26 illustrates the verification of the steady-state temperature calculator.

FIGURE 26. Verification of Steady-State Fuel Radial Temperature Profile Model

- Models used to describe separate effects, such as the thermal conductivity of fill gas, were validated by comparison to data. Figure 27 illustrates this type of validation.
- Statements on the validity of the entire code were prepared based on comparison to irradiation experiments. A series of defined tests were used in this comparison; Figure 28 provides an example of one comparison.

For each code/data comparison presented, a discussion of code usage and the experimental data were supplied to clarify and identify differences and similarities. Based on their work, the authors made the following general conclusions:

- mathematical consistency - The temperature calculations were accurate relative to analytical solutions; the mechanical models were consistent with a detailed finite element model.

FIGURE 27. Validation of Gas Thermal Conductivity Model

- individual model validation - Comparison of the major models with recognized data sets showed that the models were contributing reasonable results to the overall calculation.
- total model validation - General agreement between code and data was obtained with some exceptions (which were listed).

This validation exercise provided no concrete limits on the usage of the code, and no statistical analysis was performed on the differences between code and data.

FIGURE 28. Example of Validation of a Fuel Performance Code

The stated objectives for the assessment of FRAPCON-1 (Laats, Peeler, and Scofield 1979) were to evaluate the general code performance characteristics (model analysis) and perform a code/data comparison to evaluate model accuracy (model validation). Code verification is not presented in either the assessment document or the description document (Berna and Bohn 1980).

Model analysis of FRAPCON-1 consisted of running FRAPCON-1 and FRAP-S3 (Dearien 1978) on a selected problem, which resulted in the identification of changes in predictions due to model differences between the two codes.

To perform the FRAPCON-1 model validation, a large set of irradiation data was compiled and FRAPCON-1 predictions were obtained. Two major forms of comparison are presented: plots of prediction versus data and plots of the difference between prediction and data. The resulting plots consist of bands that can be statistically analyzed to provide error estimates for the code relative to data.

Because of the large number of code/data comparisons, the FRAPCON-1 assessment used a substantial amount of computer time compared to the GT3 verification. In addition, it becomes more difficult to provide an estimate of the quality of each individual piece of data. However, it can also be said that this type of comparison provides a fair definition of the bounds and limitations of the code.

The third example is not truly a model validation exercise but an attempt to determine which of several fuel behavior codes was better. Freeburn, Pati, and Fiero (1977) compared six codes against five sets of irradiation data. The report presents a discussion of the codes, the data, the code predictions, and an evaluation of the performance of the codes.

The method of evaluation was to observe the differences between code predictions and experimental data. The following parameters were used:

- The bias (B):

$$B = \frac{\sum W(P - E)/U}{N}$$

where P = the prediction

E = the experimental value

U = the absolute uncertainty of the experimental value

W = the relative weight (importance) of the experimental value

N = the number of comparisons.

- The standard deviation of the differences (R*):

$$R^* = \frac{\sum W \{[(P - E)/U] - B\}}{N}$$

The final ranking of the codes was based on the values of R^* by assuming that a minimum value of R^* identified the best overall code.

This method of evaluation is useful in evaluating the integral response of a code and identifying any consistent bias in the integral behavior of the code relative to the data. However, the results are highly dependent upon the choice of weighting factors and uncertainties. It is quite possible that by changing weights and uncertainties and making a minor change to one or more codes the final ranking of the codes could change. In addition, the analysis only identified the code with the minimum difference to the data. To be used as a model validation tool, it would have been necessary to specify what the minimum acceptable values of B and R^* would be.

The final validation example is different from the examples already reviewed. The three previous examples have compared code predictions to data from single rods irradiated under different conditions. There are now data available from a test assembly that had three identical rods. Thus, rather than comparing a code to data and estimated uncertainty, it is possible to compare a code to the observed variability between supposedly identical rods.^(a) An observed band of data from nominally identical conditions should provide a better basis for code validation than a band of data from known differing conditions.

In this type of comparison, the uncertainty band for the code prediction should be interpreted as follows: Given the assigned uncertainty for code input and models, experimental data would be expected to fall within the code uncertainty band if the fuel rod was behaving according to the models in the code. If the code and data bands overlap, then it may be said that the difference between code and data has a low level of significance; however, if the data and code bands do not overlap, there is a high significance to the code/data difference. It then becomes a problem of deciding if the code had the wrong input, if the data were observed incorrectly, or if the wrong models were used in the code.

(a) Obviously the rods are not truly identical. Manufacturing tolerances and localized differences in neutron flux will combine to produce slightly different response between fuel rods.

The third fuel assembly to be irradiated under the Experimental Support and Development of Single-Rod Fuel Codes Program is IFA-513 (Bradley et al. 1979). It contains three nominally identical rods of BWR design, and each rod contains two centerline thermocouples for data acquisition. Figure 29 compares the observed data from IFA-513 during its startup (Cunningham and Lanning 1978) with the predicted behavior from GT3. The variance bands on the data are calculated as

$$\bar{X} = \frac{\sum X_i}{N}$$

$$\sigma = \sqrt{\frac{\sum X_i^2 - (\sum X_i)^2 / N}{N - 1}}$$

where the X_i are the individual observations and N is the total number of observations. The uncertainty band for the code prediction is based on STORE, using input uncertainties appropriate to the Halden Boiling Water Reactor (PNL-2581).

A second code has also been run against the IFA-513 data. This code, FRAPCON-1, is the first of a new series of audit codes currently being developed and used by the Fuel Behavior Research Branch of the NRC. Figure 30 compares this code to the data. Because FRAPCON-1 attempts to account for cracked fuel effects, the following changes to STORE were necessary:

- A fuel thermal conductivity multiplier equal to that used in FRAPCON-1 was used.
- Fuel thermal conductivity uncertainty was increased to 25% to account for the uncertainty of the multiplier.

Several observations can be made from Figures 29 and 30. First, both GT3 and FRAPCON-1 overpredict the measured temperatures for IFA-513, with FRAPCON-1 predicting the higher temperatures. Second, when assuming a 10% uncertainty for fuel thermal conductivity, there is a significant difference between code predictions and observed behavior (the predicted uncertainty bands for the codes and the observed variance band for the data do not

FIGURE 29. Comparison of GAPCON-THERMAL-3 to IFA-513 Startup Data

FIGURE 30. Comparison of FRAPCON-1 to IFA-513 Startup Data

overlap). Finally, because FRAPCON-1 applies a crack factor to the fuel thermal conductivity, the uncertainty for fuel thermal conductivity was increased to 25%. With this change, the uncertainty band for FRAPCON-1 does overlap the observed variance band for the data.

It is acknowledged that this discussion has made no definitive statements on the validity of current fuel rod models. The purpose of this section has been to present the difficulties and possibilities of validating the modeling process. Examples were provided to illustrate different aspects of the discussion.

FIGURE 30. Comparison of FRAPCON-1 to IFA-213 Startup Data

CRACKED PELLETS AND UNCERTAINTY ANALYSIS

Until recently fuel modelers have made the assumption that fuel behaves as a solid right-circular cylinder concentrically located within the cladding. Although modelers have recognized that the fuel cracks, the assumption of concentric cylinders has been made for simplicity; and it has generally been adequate for thermal calculations but not always for the corresponding mechanical predictions. Because of this increasing awareness that the concentric cylinder model is limited, modeling efforts are now turning toward the problem of improving the interrelation of thermal and mechanical models. This section examines one such new model and its effect upon predicted uncertainty for temperatures and stored energy.

Macrographs of irradiated fuel have consistently shown a network of radial and circumferential cracks in the fuel. However, until recently only limited effort has been made to account for the effects those cracks may have upon the thermal and mechanical response of fuel rods. To prepare for the development of cracked pellet models, the Single-Rod Fuel Codes Program has been collecting transient temperature data for use in evaluating fuel rod behavior (Cunningham, Lanning, and Montgomery 1979). It has been concluded from model/data comparisons that a simplified cracked pellet model provides a better match with the transient temperature data than does the solid pellet model.

A cracked pellet model has been developed that utilizes "effective" values of fuel thermal conductivity and elastic modulus. These effective values are a function of the state of the fuel rod (Williford et al. 1980). This model, to be used in FRAPCON-2,^(a) has the following basic features:

- Thermal stresses cause the fuel to crack and relocate outward, thereby resulting in a smaller fuel-cladding gap than predicted by thermal expansion of a solid pellet alone.

(a) FRAPCON-2 has not yet been released; September 1980.

- Because of relocation, the fuel remains in constant contact with the cladding. The contact pressure is determined by equating the fuel hydrostatic stress to the radial stress at the gap.
- The effective fuel thermal conductivity and elastic moduli (radial and axial) are dependent on the cracks that exist within the fuel. As power and temperature increase, decreasing crack width (due to thermal expansion) increases the interaction between pellet fragments and therefore increases the effective thermal conductivity and elastic moduli.

In essence, the thermal and mechanical calculations remain based on the solid pellet model (for ease of calculation), but gap conditions and fuel properties (thermal and mechanical) are controlled by the available volume, which is in turn controlled by temperature and crack geometry.

This new model can be seen to affect uncertainty predictions in the following ways:

- Water film and cladding temperatures, and their uncertainty, are unaffected.
- The minimum value of gap conductance is equivalent to a closed gap with no interfacial pressure. Therefore, the uncertainty for gap size and gap conductance is reduced.
- The fuel thermal conductivity (K_F) is reduced by applying a multiplier (C_F) to the conductivity integral. Since there is an uncertainty for the multiplier (in addition to the uncertainty for the conductivity integral), the fuel thermal conductivity uncertainty is increased. This in turn changes the uncertainty predictions for fuel temperatures.
- The calculational method for stored energy is unchanged; however, the temperature profile and uncertainties are changed. Therefore, the predicted stored energy and its uncertainty will change.

Since by definition the thermal conductivity multiplier is the ratio of cracked pellet thermal conductivity to solid pellet thermal conductivity, it follows that the value of C_F ranges from 0.0 to 1.0. For specific values of T_S and T_{CL} , C_F is found from

$$C_F = \frac{\frac{qF}{4\pi}}{\int_{T_S}^{T_{CL}} K_F(T) dT}$$

Thus, if T_{CL} is known (data or calculation) and a minimum T_S is specified, the calculated value of C_F is a minimum (i.e., maximum thermal conductivity reduction).

Figure 31 presents minimum C_F values for BWR 8x8 and PWR 17x17 rod designs as a function of rod total thermal resistance. The principal assumptions needed to derive the curves in this figure are coolant temperature, temperature rise across the fuel-cladding gap, and power level. Table 13 lists the power, fuel surface temperature, and centerline temperature for $C_F = 1.0$. It should be recalled that an increase in resistance for a constant power means an increase in centerline temperature.

The curves in Figure 31 define the lower boundary of the interaction region between C_F and thermal resistance ($C_F = 1.0$ is the upper boundary). Since the difference in temperature between centerline and fuel surface is inversely proportional to fuel thermal conductivity (i.e., as K_F increases, $\Delta T = T_{CL} - T_S$ decreases), changes in C_F will dictate changes in fuel temperature. Thus, as C_F increases from the minimum for a constant resistance (constant centerline temperature), the fuel surface temperature will increase. On the other hand, if C_F increases and T_S is fixed, T_{CL} and thermal resistance will decrease.

The uncertainty for fuel thermal conductivity (UK_F) is a combination of the uncertainty for the solid thermal conductivity and the uncertainty for the conductivity multiplier. The total uncertainty is found from the two contributions by:

FIGURE 31. Minimum Conductivity Multiplier Values as a Function of Thermal Resistance

TABLE 13. Assumptions of Parametric Plots of Minimum C_F Versus Resistance

Rod Type	Power, kW/m	Fuel Surface(a) Temperature, K	Centerline(b) Temperature, K
BWR: $T_w = 553K$	20	619	990
	35	646	1424
	50	673	1961
PWR: $T_w = 578K$	20	642	1026
	35	667	1470
	50	693	2013

(a) Fuel surface temperature calculated assuming $\Delta T_g = 30K$

(b) $C_F = 1.0$; Lyons thermal conductivity

$$UK_F = \left(UK_{F-solid}^2 + UC_F^2 \right)^{1/2}$$

Reasonable estimates of $UK_{F-solid}$ have already been made, making the problem one of estimating the conductivity multiplier uncertainty.

In Figure 31 the upper and lower boundaries for the conductivity multiplier were developed as a function of total thermal resistance. By using these boundaries it is possible to define the maximum uncertainty for C_F . The relative uncertainty may be specified as the ratio of the difference between the maximum ($C_F = 1.0$) and minimum multiplier ($C_F = C_{F-m}$) to the assumed value of the multiplier

$$UC_F(\%) = \frac{(1 - C_{F-m})}{C_F} \cdot 100$$

Thus, for a rod with low thermal resistance and small void volume, C_F is near 1.0 and has a small relative uncertainty. For a rod with high resistance, the range of possible C_F values is larger and the relative uncertainty for the multiplier is larger.

To show the effect upon uncertainty due to cracked pellet modeling, two rod designs were evaluated. Using the BWR 8x8 and PWR 17x17 power/temperature histories discussed in the Fuel Rod Design Analysis section, three STORE runs were made:

- solid pellet: $C_F = 1.0$, varying ΔT_g , $UK_F = 10\%$
- cracked pellet: $C_F = \text{minimum}$, $\Delta T_g = 30K$, $UK_F = 10\%$
- cracked pellet: $C_F = \text{minimum}$, $\Delta T_g = 30K$, $UK_F = 20\%$.

For each run, the centerline temperature history matched that presented earlier.

The resulting centerline temperature and stored energy relative uncertainties are approximately constant with burnup; the range of values seen in Table 14 occurs throughout the burnup history. Notice that there is no overlap for the predicted relative uncertainties; and, as would be expected, the cracked pellet modeling has higher relative uncertainties predicted for centerline temperature and stored energy. In addition, relative uncertainties increase as the input fuel thermal conductivity uncertainty increases.

TABLE 14. Effect of Cracked Pellet Model on Relative Uncertainties

	% Uncertainty (3σ)	
	BWR 8x8	PWR 17x17
Centerline Temperature		
A	14.9-16.0	15.0-16.0
B	16.6-17.7	15.6-16.8
C	18.0-20.0	17.0-18.3
Stored Energy		
A	18.7-22.5	20.5-21.9
B	22.5-23.2	22.3-22.7
C	24.1-25.5	23.8-24.5

A: Solid Pellet $UK_F = 10\%$

B: Cracked Pellet $UK_F = 10\%$

C: Cracked Pellet $UK_F = 20\%$

Although the relative uncertainty for stored energy is higher for the cracked pellet model than for the solid pellet model, the upper absolute bound^(a) for stored energy is lower for the cracked pellet model. The cracked pellet, with its lower fuel surface temperature, has a lower volumetric average fuel temperature and thus a lower stored energy. In general, the stored energy is sufficiently lower for the cracked pellet so that its higher value of relative uncertainty will not result in the absolute uncertainty bound exceeding that of the solid pellet. This effect is illustrated by plotting the predicted stored energy (Figure 32) and the three associated upper absolute bounds (Figure 33) for the BWR 8x8 power history.

Obviously, it would be possible for the cracked pellet upper absolute uncertainty bound to exceed the solid pellet upper absolute uncertainty bound if larger input uncertainties are used during cracked pellet uncertainty analysis. However, the values presented here are believed to be reasonable estimates of the uncertainties for cracked pellet modeling.

In summary, a cracked pellet model has the following effects on steady-state fuel rod temperature calculations relative to a solid pellet model:

- decreased fuel surface temperature because of the increased gap conductance
- decreased stored energy because of decreased fuel volumetric average temperature
- increased relative uncertainty for fuel centerline temperature and stored energy because of increased fuel thermal conductivity uncertainty
- decreased upper absolute uncertainty because of decreased stored energy.

(a) The absolute uncertainty bound is calculated from the nominal value and relative uncertainty by: $U_x \text{ (absolute)} = X_{\text{nominal}} * [(1.0 \pm U_x \text{ (relative)})]$.

FIGURE 32. BWR 8x8 Stored Energy Based on Solid and Cracked Pellet Models

FIGURE 33. BWR 8x8 Stored Energy Upper Absolute Uncertainty Bounds

REFERENCES

- Bellamy, R. G., and J. B. Rich. 1969. "Grain-Boundary Gas Release and Swelling on High Burnup Uranium Dioxide." J. Nucl. Mat. 33:64-78.
- Beyer, C. E., and C. R. Hann. November 1974. Prediction of Fission Gas Release From UO₂ Fuel. BNWL-1875, Pacific Northwest Laboratory, Richland, Washington.
- * Bradley, E. R., et al. November 1979. Precharacterization Report for Instrumented Nuclear Fuel Assembly IFA-513. NUREG/CR-1077, PNL-3156, Pacific Northwest Laboratory, Richland, Washington.
- * Cunningham, M. E., and D. D. Lanning. July 1979. Startup Data Report for NRC/PNL Halden Assembly IFA-513. NUREG/CR-0862, PNL-2948, Pacific Northwest Laboratory, Richland, Washington.
- * Cunningham, M. E., D. D. Lanning, and S. D. Montgomery. October 1979. A Procedure for the Qualitative Interpretation of Fuel Centerline Thermocouple Response to Step-Power Decreases. NUREG/CR-1012, PNL-3096, Pacific Northwest Laboratory, Richland, Washington.
- * Cunningham, M. E., et al. May 1978. Stored Energy Calculation: The State of the Art. NUREG/CR-0320, PNL-2581, Pacific Northwest Laboratory, Richland, Washington.
- Dearien, J. A., et al. March 1978. FRAP-S3: A Computer Code for Steady-State Analysis of Oxide Fuel Rods, Volume I, Analytical Models and Input Manual. TFBP-TR-164, EG&G Idaho, Inc., Idaho Falls, Idaho.
- Freeburn, H. R., S. R. Pati, and I. B. Fiero. March 1977. Light Water Reactor Fuel Rod Modeling Code Evaluation. EPRI-NP-369, Electric Power Research Institute, Palo Alto, California.
- * Hagrman, D. L., and G. A. Reymann. February 1979. MATPRO - Version 11; A Handbook of Materials Properties for Use in the Analysis of Light Water Reactor Fuel Rod Behavior. NUREG/CR-0497, TREE-1280, EG&G Idaho, Inc., Idaho Falls, Idaho.
- * Hann, C. R., et al. November 1977. Test Design, Precharacterization, and Fuel Assembly Fabrication for Instrumented Fuel Assemblies IFA-431 and IFA-432. NUREG/CR-0332, BNWL-1988, Pacific Northwest Laboratory, Richland, Washington.
- Kerrisk, J. F., and D. G. Clifton. 1972. "Smoothed Values of the Enthalpy and Heat Capacity of UO₂." Nuclear Tech. 16:531-535.
- * Laats, E. T., G. B. Peeler, and N. R. Scofield. May 1980. Independent Assessment of the Steady State Fuel Rod Analysis Code FRAPCON-1. NUREG/CR-1339, Idaho National Engineering Laboratory, Idaho Falls, Idaho.

Lanning, D. D., et al. January 1978. GAPCON-THERMAL-3 Code Description. PNL-2434, Pacific Northwest Laboratory, Richland, Washington.

Lokken, R. O., and E. L. Courtright. 1977. A Review of the Effects of Burnup on the Thermal Conductivity on UO₂. BNWL-2270, Pacific Northwest Laboratory, Richland, Washington.

Lyons, M. F., et al. 1964. UO₂ Pellet Thermal Conductivity from Irradiation with Central Melting. GEAP-4624, General Electric Co., San Jose, California.

Mar, B. W. 1974. "Problems Encountered in Multidisciplinary Resources and Environmental Simulation Models Development." J. of Environmental Management 2:83-100.

McKay, M. D., R. J. Beckman, and W. J. Conover. May 1979. "A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code." Technometrics 21:239-245.

Mitchell, T. J., and D. G. Wilson. November 1979. Energy Model Validation: Initial Perceptions of the Process. ORNL/CSD-50, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

* Williford, R. E., et al. April 1980. Interim Report; The Analysis of Fuel Relocation for the NRC/PNL Halden Assemblies IFA-431, IFA-432, and IFA-513. NUREG/CR-0588, PNL-2709, Pacific Northwest Laboratory, Richland, Washington.

*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

APPENDIX A

THERMAL MODELS IN STORE

APPENDIX A

THERMAL MODELS IN STORE

The fuel models that are used in STORE are discussed in this appendix. Any change in modeling from PNL-2581 will be noted; however, no changes have been made that require changes to the uncertainty equations listed in Appendix B of PNL-2581.

It should be kept in mind that STORE is not a history-dependent code; therefore, history-dependent parameters such as fill gas composition must be input to STORE from the code of choice. This simplifies the workings of STORE since elaborate models are not used; only the end result and uncertainty of those models are used.

The models used in STORE are

- Water Film Temperature Rise

The temperature rise across the water film (ΔT_f) is determined by

$$\Delta T_f = \frac{q}{\pi d_{co} h_f}$$

where the water film heat transfer coefficient (h_f) and cladding outer diameter (d_{co}) are obtained from the results of each time step of the code of choice and q denotes the local linear heat rate.

- Cladding Temperature Rise

The temperature rise across the cladding (ΔT_c) is found by

$$\Delta T_c = \frac{q \ln (d_{co}/d_{ci})}{2\pi K_c}$$

where the cladding thermal conductivity (K_c) is obtained from the code of choice and d_{ci} is the cladding inner diameter.

- Cladding Inner Surface Temperature

The temperature on the cladding inner surface (T_c) is determined by summing the coolant temperature (T_w), water film temperature rise, and cladding temperature rise

$$T_c = T_w + \Delta T_f + \Delta T_c$$

- Temperature Rise Across the Gap and Fuel Surface Temperature

The temperature rise across the gap between the fuel and cladding (ΔT_g) is determined by

$$\Delta T_g = \frac{q}{\pi d_g h_g}$$

where d_g is the diameter of the gap and h_g is the gap conductance. The fuel surface temperature (T_s) is found from

$$T_s = T_c + \Delta T_g$$

Because the fuel surface temperature is determined from the temperature rise across the gap but is also required in the solution for the gap temperature rise, an iterative solution is required.

The gap conductance is defined as

$$h_g = \frac{K_g(T_g)}{x_e} + h_s$$

where $K_g(T_g)$ is the thermal conductivity of the gas in the gap evaluated at the average gap temperature (T_g), x_e is the effective gap width, and h_s is the conductance due to fuel-cladding contact. Obviously, x_e and h_s are dependent upon whether or not fuel-cladding contact has occurred.

For no fuel-cladding contact, X_e is the sum of the physical gap (X_p) and the temperature jump distance (TJ). The physical gap is defined as

$$X_p = \frac{d_{fi}}{2} \left(\sqrt{F_{pr}} - \sqrt{F_p} \right) + R$$

where d_{fi} is the initial fuel diameter, F_p and F_{pr} determine the reversible and permanent changes in fuel cross-sectional area, respectively,^(a) and R is the combined roughness of the fuel and cladding.

The temperature jump distance is defined as

$$TJ = a_g K_g (T_g) \sqrt{T_g + 273}$$

where a_g is a coefficient. The solid conductance (h_s) is zero.

For fuel-cladding contact, the effective gap width is defined as

$$X_e = (R + TJ) \exp(-C_1 \Delta F_p)$$

The solid conductance is found from

$$h_s = C_2 \Delta F_p$$

where ΔF_p is the difference between the square roots of F_p and F_{pr} . The coefficients C_1 and C_2 are determined by assuming limiting conditions for the minimum effective gap and the maximum solid conductance.^(b)

In PNL-2581, the gas thermal conductivity was determined from a cubic function that was input for each different gas mixture. To simplify the

(a) See PNL-2581 for a discussion of the derivation and meaning of F_p and F_{pr} .

(b) Minimum gap width = 0.5 R

Maximum contact conductance = 0.0015 W/m²-K

use of STORE, the KGAS subroutine from GT3 (used to calculate gas thermal conductivity) has been added to STORE. It is now necessary to input only the appropriate gas mixture, rather than determining a conductivity function.

- Fuel Centerline Temperature

With the fuel surface temperature specified, it is possible to solve for the fuel temperature at any radius through the use of the integral conductivity method. Specifically, for the fuel centerline temperature

$$\int_{T_s}^{T_{CL}} K_F(T) dT = \frac{qF}{4\pi}$$

where the fuel thermal conductivity (K_F) and flux depression (F) are the same as used in the code of choice.^(a)

- Stored Energy

The stored energy of the fuel (E_s) relative to the coolant temperature may be simply stated as

$$E_s = C_p(T_a) \left[T_a - T_w \right] \frac{\rho \pi d_{ff}^2}{4}$$

where C_p is the fuel specific heat, T_a is the fuel volumetric average temperature, ρ is the fuel density, and d_{ff} is the hot fuel diameter. This does not account for any stored energy in the cladding or fuel-cladding gap.

(a) GT3 and STORE use the thermal conductivity expression for 95% TD UO_2 developed by Lyons (1964) and modified by the Maxwell-Eucken correction for densities other than 95% TD.

APPENDIX B

THERMAL RESISTANCE

APPENDIX B

THERMAL RESISTANCE

Data from in-reactor fuel rod tests commonly consist only of power, coolant temperature, and fuel centerline temperature. As a result, only one thermal property can be determined from these parameter measurements: thermal resistance. By analogy with Ohm's Law, thermal resistance is the ratio of potential to current. More specifically, the total thermal resistance for a fuel rod is defined as the difference between the fuel centerline and coolant temperatures divided by the local linear power

$$R_T = \frac{T_{CL} - T_W}{q}$$

In a fuel rod, the total thermal resistance is the sum of resistances for the individual regions: cladding, gap, and fuel. Figure B.1 illustrates the general resistance versus power behavior for a typical boiling water reactor (BWR) fuel rod at beginning of life (BOL). The decrease in gap resistance is due to fuel thermal expansion closing the gap and increasing the gap conductance. The fuel resistance increases with power because fuel thermal conductivity decreases with temperature.

A fuel rod is classified as balanced if resistance is constant with power; fuel-dominated if resistance increases with power; or gap-dominated if resistance decreases with power (Figure B.2). As examples, a helium-filled rod with a small fuel-cladding gap will be identified as fuel dominated, while a xenon-filled rod will be identified as gap dominated. Resistance versus power plots are therefore useful tools in inferring fuel rod behavior.

FIGURE B.1. Components of Resistance

FIGURE B.2. Resistance Behavior of Various Rods

Since T_{CL} , T_W , and q are all separately measured during experiments, there are no covariances between these parameters; and the relative variance for resistance calculated from data may be found from

$$\sigma_{R_T}^2 = \sum_{i=1}^p \left(\frac{\partial R_T}{\partial X_i} \right)^2 \sigma_i^2$$

where the X_i are the variables T_{CL} , T_W , and q , and the σ_i^2 are their variances. Relative variance may be defined as

$$C_i^2 = \frac{\sigma_i^2}{\mu_i^2}$$

where μ_i is the mean value of X_i . The relative variance of the thermal resistance may be written as

$$C_{R_T}^2 = \frac{T_{CL}^2}{(T_{CL} - T_W)^2} C_{T_{CL}}^2 + \frac{T_W^2}{(T_{CL} - T_W)^2} C_{T_W}^2 + C_q^2$$

The percent uncertainty ($3\sigma = 99.7\%$ confidence level) for experimentally measured thermal resistance is then

$$U_{R_T} = 300 \sqrt{C_{R_T}^2}$$

Since T_{CL} , T_W , and p are all separately measured during experiments, there are no covariances between these parameters; and the relative variance for resistance calculated from data may be found from

$$\sigma_{RT}^2 = \sum_{i=1}^p \left(\frac{\partial R}{\partial X_i} \right)^2 \sigma_{X_i}^2$$

where the X_i are the variables T_{CL} , T_W , and p , and the $\sigma_{X_i}^2$ are their variances. Relative variance may be defined as

$$C_R = \frac{\sigma_R^2}{\bar{R}^2}$$

where $\bar{R}$ is the mean value of R . The relative variance of the thermal resistance may be written as

$$C_{RT}^2 = \frac{C_{T_{CL}}^2}{(T_{CL} - T_W)^2} + \frac{C_{T_W}^2}{(T_{CL} - T_W)^2} + C_p^2$$

The percent uncertainty (3σ = 99.7% confidence level) for experimentally measured thermal resistance is then

$$U_{RT} = 300 \sqrt{C_{RT}^2}$$

APPENDIX C

BURNUP-DEPENDENT FILL GAS COMPOSITION

APPENDIX C

BURNUP-DEPENDENT FILL GAS COMPOSITION

This appendix provides a brief presentation of the change in fuel rod fill gas composition during burnup. Figures C.1 to C.5 present the change in gas composition that was predicted by GT3 for the Case 2 power histories discussed in the Fuel Rod Design Analysis section. The solid line in each figure is the predicted composition, and the dotted lines are the upper and lower composition boundaries based on the 1% estimate for gas release uncertainty. Figure C.6 illustrates the change in gas thermal conductivity that occurs as an increasing amount of fission gas (xenon and krypton) is mixed with the original helium. Note that as the percentage of fission gas increases, the rate of change of thermal conductivity decreases.

The results presented in Figures C.1 to C.5 were combined with Figure C.6 and used to determine gas thermal conductivity uncertainty for each burnup step (see Table 6 in text). It can be seen that the boiling water reactor (BWR) rods (Figures C.1 to C.3) have a possible wide variation in gas composition at a specific burnup and thus a large thermal conductivity uncertainty. At higher burnups the composition band begins to narrow, and the thermal conductivity curve is flatter; therefore, thermal conductivity uncertainty at end-of-life (EOL) is lower. On the other hand, the larger initial amounts of helium in the pressurized water reactor (PWR) rods counteract fission gas release and result in a narrower gas composition band throughout the power history (Figures C.4 and C.5). Thus, the PWR rods have a lower gas thermal conductivity uncertainty.

FIGURE C.1. Fill Gas Composition History for BWR 7x7, Case 2

FIGURE C.2. Fill Gas Composition History for BWR 8x8, Case 2

FIGURE C.3. Fill Gas Composition History for 3 atm BWR 8x8, Case 2

FIGURE C.4. Fill Gas Composition History for PWR 15x15, Case 2

FIGURE C.5. Fill Gas Composition History for PWR 17x17, Case 2

FIGURE C.6. Gas Thermal Conductivity as a Function of Fill Gas Composition at 673K

DISTRIBUTION

<u>No. of Copies</u>		<u>No. of Copies</u>	
<u>OFFSITE</u>		<u>ONSITE</u>	
	A. A. Churn DOE Patent Division 9300 S. Cass Avenue Argonne, IL 60439	46	<u>Pacific Northwest Laboratory</u>
400	Nuclear Regulatory Commission Division of Technical Information and Document Control 7920 Norfolk Avenue Bethesda, MD 20014		W. J. Bailey J. O. Barner E. R. Bradley M. E. Cunningham (20) S. K. Edler M. D. Freshley R. L. Goodman R. J. Guenther C. R. Hann K. A. Hsieh D. D. Lanning R. K. Marshall C. L. Mohr C. Nealley A. R. Olsen F. E. Panisko W. N. Rausch R. E. Schreiber R. E. Williford Technical Information (5) Publishing Coordination Fe(2)
2	DOE Technical Information Center		
4	W. V. Johnston Chief, Fuel Behavior Research Branch Division of Reactor Safety Research U.S. Nuclear Regulatory Commission Washington, D.C. 20555		
	H. H. Scott Fuel Behavior Research Branch Division of Reactor Safety Research U.S. Nuclear Regulatory Commission Washington, D.C. 20555		

WUREG/CR-1753
PWL-2230
R-3

DISTRIBUTION

No. of Copies	No. of Copies	<u>OFFSITE</u>	<u>ONSITE</u>
		A. A. Churn DOE Patent Division 9500 S. Cass Avenue Argonne, IL 60439	46 Pacific Northwest Laboratory
		400 Nuclear Regulatory Commission Division of Technical Information and Document Control 7950 Norfolk Avenue Bethesda, MD 20014	W. J. Bailey J. O. Barner E. R. Bradley M. E. Cunningham (20) S. K. Elder M. O. Freshney R. L. Goodman R. J. Guenther C. R. Hann K. A. Hester D. D. Lanning R. K. Marshall C. L. Mohr C. Westley A. R. Olsen F. E. Pankosko W. H. Rausch R. E. Schreiber R. E. Williford
		2 DOE Technical Information Center	
		4 W. V. Johnston Chief, Fuel Behavior Research Branch Division of Reactor Safety Research U.S. Nuclear Regulatory Commission Washington, D.C. 20555	Technical Information (2) Publishing Coordination (2)
		H. H. Scott Fuel Behavior Research Branch Division of Reactor Safety Research U.S. Nuclear Regulatory Commission Washington, D.C. 20555	

NRC FORM 335 (7-77)		U.S. NUCLEAR REGULATORY COMMISSION BIBLIOGRAPHIC DATA SHEET		1. REPORT NUMBER (Assigned by DDC) NUREG/CR-1753 PNL-3539	
4. TITLE AND SUBTITLE (Add Volume No., if appropriate) Application of Linear Propagation of Errors to Fuel Rod Temperature and Stored Energy Calculations				2. (Leave blank)	
				3. RECIPIENT'S ACCESSION NO.	
7. AUTHOR(S) M.E. Cunningham, A.R. Olsen, D.D. Lanning, R.E. Williford				5. DATE REPORT COMPLETED MONTH YEAR September 1980	
9. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code) Pacific Northwest Laboratory P.O. Box 999 Richland, Wa. 99352				DATE REPORT ISSUED MONTH YEAR October 1980	
				6. (Leave blank)	
				8. (Leave blank)	
12. SPONSORING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code) Division of Reactor Safety Research Office of Nuclear Regulatory Research U.S. Nuclear Regulatory Commission Washington, D.C. 20555				10. PROJECT/TASK/WORK UNIT NO.	
				11. CONTRACT NO.	
13. TYPE OF REPORT			PERIOD COVERED (Inclusive dates)		
15. SUPPLEMENTARY NOTES				14. (Leave blank)	
16. ABSTRACT (200 words or less) <p>Linear propagation of errors evaluates modeling uncertainty by approximating a function of interest by first-order Taylor's series expansions and then approximating the variance of the function by the variance of the linear approximation. This report discusses uncertainty analysis for different nuclear fuel rod designs, the process of model validation, and the effect of cracked pellet fuel models upon temperature uncertainty.</p> <p>Using a postulated power history, the uncertainty for the predicted thermal response of boiling water reactor (BWR) and pressurized water reactor (PWR) fuel rods was evaluated. Beginning-of-life (BOL) relative uncertainty for BWR and PWR fuel rods is approximately the same, while different end-of-life (EOL) thermal response results in different EOL uncertainty. Determining the validity of modeling relative to reality is discussed in qualitative terms.</p>					
17. KEY WORDS AND DOCUMENT ANALYSIS			17a. DESCRIPTORS		
17b. IDENTIFIERS/OPEN-ENDED TERMS					
18. AVAILABILITY STATEMENT Unlimited			19. SECURITY CLASS (This report) Unclassified		21. NO. OF PAGES
			20. SECURITY CLASS (This page)		22. PRICE \$

1. REPORT NUMBER NUREG-1783 PNC-3532		2. REPORT TITLE Application of Linear Propagation of Errors to Fuel Rod Temperature and Stored Energy Calculations	
3. AUTHOR(S) M.E. Cunningham, A.R. Olsen, D.O. Lanning, R.C. Whitford		4. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS Pacific Northwest Laboratory P.O. Box 999 Richland, WA 99352	
5. DATE REPORT COMPLETED MONTH: September YEAR: 1980		6. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS (If Different) Division of Reactor Safety Research Office of Nuclear Regulatory Research U.S. Nuclear Regulatory Commission Washington, D.C. 20555	
7. DATE REPORT ISSUED MONTH: October YEAR: 1980		8. PERFORMING ORGANIZATION NAME AND MAILING ADDRESS (If Different) Division of Reactor Safety Research Office of Nuclear Regulatory Research U.S. Nuclear Regulatory Commission Washington, D.C. 20555	
9. PROJECT FUNDING NUMBERS NO. 1: CONTRACT NO.		10. TYPE OF REPORT 11. SUPPLEMENTARY NOTES	
12. ABSTRACT Linear propagation of errors evaluated modeling uncertainty by approximating a function of interest by first-order Taylor's series expansion and then approximating the variance of the function by the variance of the linear approximation. This report discusses uncertainty analysis for different nuclear fuel rod designs, the process of model validation, and the effect of cracked pellet fuel models upon temperature uncertainty.		13. KEY WORDS AND SUBJECT ANALYSIS	
14. DISTRIBUTION STATEMENT UNCLASSIFIED		15. SECURITY CLASSIFICATION UNCLASSIFIED	