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**FMODEL — A FORTRAN IV COMPUTER CODE
TO PREDICT IN-REACTOR BEHAVIOR OF
LMFBR FUEL PINS**

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UC-79b -- Liquid Metal Fast Breeder Reactors
(Fuels and Materials Engineering and Development)

METALS AND CERAMICS DIVISION

F. J. Homan W. J. Lackey C. M. Cox

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FMODEL - A FORTRAN IV COMPUTER CODE TO PREDICT
IN-REACTOR BEHAVIOR OF LMFBR FUEL PINS

F. J. Homan W. J. Lackey C. M. Cox*

ABSTRACT

A computer code to predict the in-reactor behavior of stainless-steel-clad (U,Pu)O₂ fuel pins is described. The code is an integration of three complex models describing the thermal, mechanical, and chemical performance of LMFBR-type fuel pins. This report is intended to serve two purposes: (1) to acquaint the casual reader with the general methodology used in the code, and to provide comparison between predicted fuel pin performance and performance measured directly from irradiation experiments; and (2) to serve as a user's guide for readers who wish to use the code. Accordingly, general descriptions are contained in the body of the report, and detailed accounts of individual models, glossaries of variable names, and descriptions of individual subroutines are contained as appendices.

INTRODUCTION

Fuel performance modeling was one of the tasks included in the Oak Ridge National Laboratory (ORNL) program for the development of fast breeder reactor (FBR) fuels. The modeling work had several objectives. The first, of course, was to develop the means to analytically predict how a fast reactor fuel pin will behave in service, particularly when it will fail. Secondary objectives included providing guidance for the planning of irradiation tests for the program and interpretation of the results from these tests. In addition, the models were used to establish the sensitivity of fuel performance to different material properties and operating parameters. It was hoped that this would enable us to use our research money more effectively, in reducing the uncertainty in the most critical areas.

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The fuel model (FMODEL) computer code was written to predict the in-reactor performance of a single LMFBR fuel pin consisting of pelletized oxide fuel clad with stainless steel. The code is sufficiently flexible that performance of other types of fuel pins can also be predicted. For example, the irradiation behavior of a fuel pin in a thermal flux can be modeled, and pins clad with materials other than stainless steel can be analyzed with a few minor modifications to the code. FMODEL could be used for carbide and nitride fuels, but changes in the built-in fuel properties will be necessary for such use. The code can also be used for particulate fuel forms, including powders, shards, and microspheres such as those loaded by the Sphere-Pac process developed at ORNL.

This report has been prepared to give the average reader a brief description of the manner in which the FMODEL code is constructed, and to show a comparison of predicted fuel pin behavior with experimentally measured behavior in actual irradiation tests. It is also intended that this report be useful to individuals who would like to adapt the code to their own uses. Glossaries of common variables and input are contained as Appendices A and B, followed by detailed descriptions of individual phenomenological models and subroutines in Appendices C, D, E, and F.

GENERAL

FMODEL represents an integration of three fairly complex models: a thermal and heat transfer model, a fuel and cladding mechanical model, and a chemical performance model. The thermal and heat transfer model is similar to that described in the write-up of the PROFIL code,¹ except that the empirical restructuring model has been replaced with a time-dependent pore migration model based on a vaporization-condensation mechanism. The details of the restructuring model are given in Appendix C. A sophisticated model has been recently developed² to calculate the conductance of heat across the fuel-cladding gap. Total gap conductance is viewed in the model as the sum of a conductance term from solid-solid contact (when the gap has closed from differential thermal expansion or fuel swelling) and from heat transport across a gas phase separating the fuel and cladding. Accommodation effects are

considered, as well as the changing conductivity of the gas in the gap from the introduction of fission gases into the plenum during irradiation.

The mechanical model utilizes a generalized plane strain, finite difference approach. The code user can supply his own plasticity equations and creep equations to describe both thermal and flux-enhanced cladding creep. The mechanical model is applied to the fuel in a somewhat different manner than to the cladding, because of the extreme plasticity of the central portion of the fuel and because of the cracks that form in the cooler fuel regions. The mechanical model has been incorporated into a fuel cracking model, which is described in Appendix F under SUBROUTINE PLAST. The details of the mechanical model are given in Appendix E.

The chemical model describes the transport of oxygen, uranium, and plutonium during irradiation. Thermodynamic considerations are employed in these calculations, and the results are extremely sensitive to the initial oxygen-to-metal ratio of the fuel. The details of this model have recently been published³ and will not be repeated in this report. Component redistribution is very important in a performance model because of the influence of plutonium content and stoichiometry on thermal conductivity, thermal expansion, the melting temperature, and the creep characteristics of mixed oxide fuels. Failure to account for these changes will result in a model that does not properly compute temperature changes with irradiation and can lead to serious errors in other performance characteristics.

The general approach used in FMODEL is to divide the fuel pin into a user-specified number of axial regions, with each axial region further divided into concentric rings. Then the performance of each region at an axial node located in the axial center of the region is calculated. The irradiation history of interest is broken down into components or cycles, and the performance of each axial node is calculated in turn for each cycle. This process is repeated until all cycles have been completed. Thus two noding systems are required — axial and radial. Storage locations are required to store the performance calculations from one axial node while calculations are being performed on other nodes. At the end of each cycle the performance information can be output for examination. The code user has complete control of the amount of information output.

Performance calculations at a given axial node begin with the temperature distribution in the fuel and cladding, based on fuel and cladding geometry and reactor operating conditions. Mechanical and physical properties are then determined for each fuel and cladding node, based on the temperature, porosity, grain size, and other parameters for the fuel or cladding at that node. The temperatures and properties calculated are assumed to remain constant for a time period Δt . The length of Δt is under the control of the code user. The continuously changing real-life situation can be approximated more closely by making Δt small, but a penalty is paid in greater computer time requirements. During any Δt both the fuel and cladding will be subjected to various types of stresses. Both will have a temperature gradient, fission gas pressure, and perhaps pressure due to fuel-cladding mechanical interaction. In addition, both will swell, the cladding because of void formation and the fuel because solid fission products and retained fission gas accumulate in its lattice. The geometry changes brought about by response to the fuel and cladding stresses are calculated at the end of each time period, and the temperature distribution is recalculated. Then the physical and mechanical properties are redetermined and the process repeated until the entire time period of interest has been covered.

Changes in power are modeled as occurring stepwise. A linear power ramp is replaced by a series of vertical steps, followed by horizontal periods of constant power. The number of such steps in a given power change is under the control of the user. The code has been designed to follow the broad changes in reactor power history with the characteristics of each cycle input. However, if the detailed power history is to be followed it is more convenient to merely read in the reactor power as a function of time and write a small routine to generate the other necessary cycle characteristics. See Appendix B for a description of the cycle characteristics required.

Several assumptions and simplifications are inherent in the FMODEL code. A listing and brief discussion of each is given below.

1. The heat transfer analysis considers heat flow in the radial direction only. The axial length is divided into a user-specified number of regions, for which the calculations representing the entire region

are performed for the axial midpoint of the region. Axial heat flow near the ends of the rod probably causes a temperature distribution in those regions somewhat different than that calculated with the one-dimensional analysis at the region midpoint. This effect is ignored in the present version of the code.

2. The cladding mechanical analysis assumes circumferential symmetry as well as plane strain. Thus the effects of cladding bowing due to asymmetrical distributions of neutron flux and coolant temperature are ignored. Similarly, the stress effects due to the presence of wire wrap or grid spacers are ignored. Friction forces between fuel and cladding are also ignored.

3. One simplification used in the code is to neglect time-dependent cladding wastage. This is somewhat difficult to treat analytically because the nature of intergranular penetration of fission products at the cladding inner surface is such that the cladding strength may be lost, but its volume is still present to influence fuel-cladding mechanical interaction. In addition, swelling and plastic strain are being accumulated as functions of time and radial position across the cladding. If cladding nodes are "disappearing" because of wastage, it is difficult to keep track of these quantities. Therefore, our present position is that because of the lack of data and understanding concerning this effect, it is better to make allowances for wastage in the initial cladding thickness than to attempt to describe the wastage phenomenon as a time-dependent event.

4. Cladding creep and tensile properties are presently treated in the code as independent of plastic strain and irradiation. It is well-known qualitatively that annealed claddings harden and cold worked claddings soften from irradiation, and it would be a simple matter to substitute quantitative relationships to describe the changes when such relationships are available.

5. Fuel creep is expressed in the code as a function of temperature, porosity, stress and grain size. Equations for UO_2 developed by Bohaboy⁴ are used for fuel with density greater than 92% theoretical, and by Clauer⁵ for fuel with densities below this value. Again, it is well-known qualitatively that the fissioning event, substitution of plutonium for uranium,

stoichiometry, porosity form, and plutonium concentration will influence creep strength in the fuel, and it is a simple matter to use suitable equations for the fuel under consideration when such quantitative relationships are available.

COMPARISON OF PREDICTION WITH EXPERIMENT

The veracity of any model is of course determined by comparing its predictions with measured behavior of the real-life system being modeled. Each of the individual models (mechanical, thermal, and chemical) contained in the FMODEL code has been thoroughly confirmed by comparing prediction with experimental measurement. It should be emphasized at this point that FMODEL contains no adjustable parameters for artificially "fitting" predicted performance to measured performance. Predicted performance depends only on the fabrication data and irradiation conditions input, the thermophysical and mechanical properties of the fuel cladding, and the validity of the models. If agreement with experimental results is not satisfactory the reason is sought in erroneous data, faulty assumptions, or omission of an important factor from the model.

Measured performance of fuel pins irradiated under fast flux conditions is presently limited to what can be observed during postirradiation examination. This is because instrumentation is very limited in EBR-II, the only fast reactor in this country in which a substantial number of mixed-oxide pins have been irradiated. In-test data can be obtained from irradiation tests in several thermal flux facilities. Although it is recognized that thermal flux tests are generally unsuitable for proof tests of fast reactor fuel elements, such tests can be valuable for understanding certain aspects of fuel performance. Pending the availability of instrumented test data from fast reactors, we have utilized thermal flux test data to test the accuracy of our thermal performance models. Fast flux test data were used for the comparison between predicted and measured diametral expansion.

Comparisons between predicted and measured performance are divided into the five areas (1) diametral expansion of the pins, (2) fuel radial

porosity distributions, (3) diameters of central void, columnar, and equiaxed-grain regions, (4) fuel center-line temperatures, and (5) uranium and plutonium redistribution.

Diametral Expansion

Permanent diametral expansion of an irradiated fuel pin is due to cladding density decrease from void formation, plastic strain accumulated throughout irradiation, and elastic strain present at room temperature due to fission gas pressure and cladding swelling gradients. Predicted diametral expansions are sensitive to the assumed cladding strength and pin fabrication and operating conditions.

Figure 1 summarizes some early FMODEL analyses on diametral expansions of several pins from the General Electric F-2 series irradiation experiments⁶ in EBR-II. Irradiation-enhanced creep of the cladding was not considered in the calculations reflected in this figure, and the August 1969 version of the WARD-PNL cladding swelling correlation⁷ was used. Mechanical interaction on startup due to differential thermal expansion between fuel and cladding was predicted for F2Q and F2H. Notice that the greatest measured diametral expansion for both these pins occurred at the cold end (bottom), where the fuel and cladding differed most in thermal expansion.

Two of the pins shown in Fig. 1, F2Z and F2H, were included in the modeling round-robin exercise.⁸ The measured and predicted diametral expansions for these pins are compared in more detail in Figs. 2 and 3. Calculations performed with the data provided for this exercise agreed far better with measurement for F2Z than for F2H. However, we have noted⁸ that both the heat rate and neutron fluence provided in the round-robin data package were below those reported in the literature for F2H. These effects account for part of the bias between observed and predicted diametral expansion for this pin.

Figure 4 compares predicted and measured diametral expansions for fuel pin F2S. This pin is particularly interesting because the fabricated smear density and heat rate were high, the fuel was axially restrained,

Fig. 1. Postirradiation profilometer traces for five fuel pins from General Electric F-2 series.

Fig. 2. Comparison of predicted and measured diametral expansions for pin F22.

Fig. 3. Comparison of predicted and measured diametral expansions for pin F2H.

Fig. 4. Comparison of predicted and measured diametral expansions for pin F2S as a function of axial position.

and the cladding was 30 mils thick. The postirradiation profilometer trace for F2S indicates a greater diametral expansion at the hot end of the pin than at the cold end. Recall that this is opposite to the observations made for F2H and F2Q. It has been suggested⁹ that the axial restraint at the top of F2S prevented any axial movement of fuel in that portion of the pin, whereas the fuel at the bottom of the pin, being more remote from the restraint, may have been freer to move axially. Our analysis supports this hypothesis. Two sets of assumptions were made in calculating the predictions plotted in Fig. 4. First, we assumed that thermal expansion and swelling of the fuel occurred isotropically; then we assumed there was complete axial restraint in all regions of the pin. Good agreement between prediction and measurement was achieved at the bottom of the pin using the isotropic assumption and at the top of the pin using the axial restraint assumption.

All comparisons between predicted and measured fuel pin diametral expansion are summarized graphically in Fig. 5. Each point of the plot

Fig. 5. Summary of comparison between predicted and measured cladding diametral expansions.

represents one axial position for the pin indicated. The measured values are the average of the 0 and 90° profilometer traces. The predicted values are those plotted on the previous figures, with the exception of F2S. The predicted values for this pin were based on the isotropic assumption at the bottom of the pin and the axial restraint assumption at the top of the pin. With the exception of pin F2H, where the actual operating conditions were uncertain, agreement is excellent. Even in this case the agreement was within 30%. Exact agreement for any pin must be considered fortuitous since the cladding density changes generally accounted for at least half the predicted diametral expansions, and the data from which the swelling correlations were derived have a wide scatter band.

Fuel Radial Porosity Distribution

FMODEL utilizes a continuous, time-dependent fuel restructuring model adapted¹⁰ from Nichols' equation¹¹ for pore motion by a vaporization-condensation mechanism. One measure of the validity of such a model is the comparison of predicted and measured void diameters and diameters of the columnar and equiaxed-grain regions. However, a difficulty with such comparisons is that axial movement of fuel will influence the measured diameters and thus distort the comparison. In addition, columnar and equiaxed grains are not exact indicators of the porosity present in a given fuel region. Therefore, actual comparison of predicted and measured radial porosity distributions in the fuel provides a much sounder basis for judging the usefulness of this model. Unfortunately, few systematic measurements of radial porosity distributions of pins irradiated under fast flux conditions are reported in the literature. Lackey and Kegley¹² measured the radial porosity distribution for a Sphere-Pac fuel pin operated at 13.6 kW/ft to about 0.7% FIMA in the Engineering Test Reactor (ETR). A postirradiation metallographic cross section of this pin is shown in the center portion of Fig. 6, and their porosity distribution data are shown in the upper portion of the figure. The solid curve shown on the upper portion of the figure is the porosity distribution predicted by FMODEL. The agreement between prediction and experiment here is excellent, except that FMODEL overpredicts the size of the central void at this axial location by about 10%.

Fig. 6. Comparison of measured and predicted porosity and $\text{Pu}/(\text{U}+\text{Pu})$ profiles.

Actinide Redistribution

The model to describe actinide redistribution is interrelated with the porosity redistribution model. We consider an axial segment of the fuel pin of unit length. After calculation of the radial temperature profile, it and the overall oxygen-to-metal ratio of the fuel are used to calculate the oxygen-to-metal distribution according to a previously proposed irreversible thermodynamic approach.¹³ Next, the porosity of each radial increment at the end of a short time period is determined from knowledge of the initial porosity and calculation (see Appendix C) of the movement of pores, or equivalently the movement of material, into and out of each radial increment. Similarly, since the initial Pu/(U+Pu) ratio for each radial increment and the amount of fuel transported into and out of each increment are known, the Pu/(U+Pu) ratio of each increment at the end of the time period can be calculated if the composition of the transported vaporous material is known. This composition was calculated³ by equilibrium thermodynamics as a function of the temperature, oxygen-to-metal ratio, and Pu/(U+Pu) ratio of the solid fuel. Repeating the calculations for a series of time periods spanning the irradiation time can give the porosity, actinide, and oxygen radial profiles at any desired time.

Predicted and measured actinide redistribution for the fuel pin discussed previously are compared in the bottom portion of Fig. 6. The agreement is very good, supporting the validity of the models used to make this calculation.

Diameters of Central Void, Columnar, and Equiaxed-Grain Regions

As mentioned earlier, another measure of the validity of any fuel restructuring model is the comparison between predicted and measured void diameters and diameters of the columnar and equiaxed-grain regions. Although this comparison is not as useful as one between predicted and measured radial porosity distributions, considerably more data are available. Predictions with measurements reported⁶ for General Electric F2

series irradiations are summarized in Fig. 7. The beginning-of-life heat rates for the pins considered ranged from 9.7 to 17.4 kW/ft, and the fabricated fuel densities ranged from 83.8 to 98.2% of theoretical. It should be emphasized that FMODEL does not predict columnar and equiaxed regions as such. Rather, it predicts porosity distributions. The columnar region has been arbitrarily assigned as any portion of the fuel with less than 2% porosity. Similarly, the equiaxed region has been arbitrarily assigned as the region between the columnar region and the region of as-fabricated density.

The results presented in Fig. 7 indicate that FMODEL somewhat overpredicts fuel restructuring. This conclusion is reached through the observation that most of the plotted points lie above the diagonal line, and it is in agreement with the discussion and results presented in the section on radial porosity distributions. Recall that in the upper portion of Fig. 6 the predicted central void was some 10% larger than the experimentally measured void.

Fig. 7. Summary of comparisons between predicted diameters for central void, columnar, and equiaxed-grain regions.

We feel that the present model is a significantly better approximation of fuel restructuring than the three-zone empirical model we have used in the past.¹⁴ The ability to predict fuel restructuring on a time-dependent basis is particularly necessary when related to the need to determine fuel-cladding mechanical interactions due to differential thermal expansion during startup. Using the earlier three-zone model we would assume that restructuring occurred "instantaneously" and would thereby underestimate the thermal expansion of the fuel and plastic deformation of the cladding.

Fuel Center-Line Temperatures

Irradiation experiments in which fuel center-line temperatures are measured have not yet been conducted with (U,Pu)O₂ fuel pins in the limited instrumented facilities available in EBR-II. Therefore, we have used thermal reactor data to test the heat generation and transfer portion of the FMODEL code. Fitts¹⁵ recently completed irradiation in the ORR of an instrumented capsule that contained 82%-smear-density (U,Pu)O₂ Sphere-Pac and pellet fuel pins in tandem. Variable heat rates were achieved by moving the capsule to different flux positions within the ORR poolside facility. Fuel center-line temperatures, cladding surface temperatures, and fuel pin heat generation rates were continuously measured and recorded during the 109 days in-reactor.

Data points representing the entire range of heat rates from 0 to 16 kW/ft were selected randomly for each pin. Using the measured cladding surface temperatures and a radial power distribution predicted by the ANISN¹⁶ neutron transport code, we calculated fuel center-line temperatures with FMODEL for both the Sphere-Pac and pellet pins. Calculated and measured fuel center-line temperatures are compared in Fig. 8.

Examination of Fig. 8 reveals that, in general, good agreement between predicted and measured fuel center-line temperatures was achieved for the Sphere-Pac fuel. However, several measured data points between 14 and 16 kW/ft appear to be low on the temperature scale. The agreement between predicted and measured pellet center-line temperatures above 9 kW/ft is poor. Because of this poor agreement, and because Fitts¹⁷

Fig. 8. Comparison between predicted and measured fuel center-line temperature variation with heat rate for pellet and Sphere-Pac pins in capsule SG-3.

suspected that one or more of the four calorimeter thermocouple pairs used to measure the heat generation rate may have been giving erroneous readings and thereby affecting the average heat generation rates plotted, a rigorous statistical analysis was performed on the SG-3 data to see if any of the data points can be justifiably discarded. The techniques and results of the statistical analysis have been reported in several sources.¹⁸⁻²¹

In the SG-3 experiment thermocouple readings were automatically recorded for 3 min every 4 hr and whenever a change in power was made. This procedure yielded 44,500 data sets or over one million recorded thermocouple readings. The temperature vs heat rate plots shown in Fig. 8 were generated from randomly selected sets of data. The statistical analysis mentioned earlier revealed that much of the data taken during startups, shutdowns, power changes, and periods when the SG-3

experiment was being markedly influenced by adjacent experiments did not follow the same trends of center temperature vs heat rate that were observed during extended periods of operation at constant heat rate. When these data are eliminated from consideration, the center temperature vs heat rate relationships for the pellet and Sphere-Pac pins from the SG-3 capsule are as shown in Fig. 9. Notice the excellent agreement between the FMODEL predictions (solid lines in Fig. 8) and the statistically verified center temperature vs heat rate curves shown in Fig. 9. It should be emphasized that the analysis shown in Fig. 8 was done in March 1971, and the statistical analysis culminating in Fig. 9 was not completed until February 1972. This demonstrates graphically one of many instances where use of FMODEL rendered great assistance in the interpretation of the data from an irradiation experiment.

Fig. 9. Statistically verified fuel central temperatures as functions of heat generation rate for capsule SG-3.

DISCUSSION

The FMODEL fuel pin performance code described in this report has proven to be a valuable tool for planning and design of irradiation experiments and interpretation of data from the experiments. The code contains models to describe most of the phenomena known to occur in an operating fuel pin. Some of the models are derived from first principles, whereas others are empirical or semiempirical. The overall calculational framework is logically and efficiently laid out so that individual models can be replaced when more sophisticated models are available. The code has been able to reasonably reproduce experimental measurements without the use of adjustable parameters to force fit code predictions to experimental observations. The code is flexible, containing many user options to attain the degree of analytical detail desired. The code requires about 300 K of core storage on the IBM 360/91 computer, and running times are under 10 min for most cases of interest. Most of the cases run to date have included 9 axial nodes, 20 fuel nodes, 5 cladding nodes, and 2 to 5 time cycles. Running times could be substantially reduced (to less than 1 min) for cases with fewer nodes and cases where fuel and cladding do not mechanically interact.

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APPENDIX A

GLOSSARY OF COMMON VARIABLES

The variables that are contained in the labeled COMMON statements are described in this appendix. The order in which the COMMON statements are considered is given below:

1. INCR	20. BURN
2. INCR2	21. SIGEPS
3. INCR3	22. CYCLE
4. TWOD	23. REDIST
5. TWOD1	24. EAMU
6. TWOD2	25. CPUMIN
7. TWOD3	26. AOUT
8. TWOD4	27. ONE
9. TWOD5	28. TWO
10. TWOD6	29. TWOX
11. START	30. THREE
12. TD1	31. THREEEX
13. INF1	32. FOUR
14. INP2	33. FIVE
15. INP3	34. SIX
16. STORE1	35. SEVEN
17. STORE2	36. EIGHT
18. STORE3	37. NINE
19. HYDRO	

<u>Name</u>	<u>Unit</u>	<u>Definition</u>
1. COMMON/INCR/		
R(I)	cm	Radius of inner boundary of <i>i</i> th increment
T(I)	°C	Temperature at inner boundary of <i>i</i> th increment
D(I)		Fractional density of fuel in <i>i</i> th increment, based on density (g/cm ³) of 100%-dense material
P(I)		Fractional porosity of fuel in <i>i</i> th increment, based on volume of pores compared to volume of fuel
F(I)	fissions cm ⁻³ sec ⁻¹	Fission rate in <i>i</i> th increment

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<u>Name</u>	<u>Unit</u>	<u>Definition</u>
2. COMMON/INCR2/		
Q(I)	W/cm	Linear heat generation rate of fuel in i th increment
A(I)	W/cm	$\int_{T_{i+1}}^{T_i} K(T) dT$
W(I)	W/cm	Linear heat rate at i th radial position (inner boundary of i th increment)
U(I)	W cm ⁻¹ °C ⁻¹	Thermal conductivity of fuel at i th radial position
SW(I)	W/cm ³	Volume heating rate of fuel in i th increment
AREA(I)	cm ²	Cross sectional area of i th increment
3. COMMON/INCR3/		
G(I)	°C/cm	Temperature gradient at the i th node
4. COMMON/TWOD/		
RADI(I,J)	cm	Radial location of the i th node in the j th axial region
DENS(I,J)		Fractional density of fuel at i th node in j th axial region
AZERO(I,J)	cm ²	Initial cold cross sectional area of i th radial increment of j th axial region
5. COMMON/TWOD1/		
XSIGR(I,J)	psi	Radial stress at i th cladding node in j th axial region
XSIGT(I,J)	psi	Tangential stress at i th cladding node in j th axial region
XSIGZ(I,J)	psi	Axial stress at i th cladding node in j th axial region

<u>Name</u>	<u>Unit</u>	<u>Definition</u>
6. COMMON/TWOD2/		
XEPR(I,J)		Plastic radial strain accumulated at <i>i</i> th cladding node in <i>j</i> th axial region
XEPT(I,J)		Plastic tangential strain accumulated at <i>i</i> th cladding node in <i>j</i> th axial region
7. COMMON/TWOD3/		
XRADI(I,J)	cm	Initial radius of <i>i</i> th node in <i>j</i> th axial region (cold)
8. COMMON/TWOD4/		
DEGC(I,J)	°C	Temperature at <i>i</i> th node in <i>j</i> th axial region
9. COMMON/TWOD5/		
GS(I,J)	μm	Grain size of fuel at <i>i</i> th radial node in <i>j</i> th axial region
10. COMMON/TWOD6/		
DEPL(I,J)	fissions/cm ³	Depletion in <i>i</i> th radial node in <i>j</i> th axial region
11. COMMON/START/		
RSTART(I)	cm	Initial cold radius of the <i>i</i> th cladding node
12. COMMON/TD1/		
EPS	cm	The effective width of the gas gap between fuel and cladding when fuel and cladding are in contact. EPS is defined by the denominator term on the right-hand side of the equals sign in Eq. (25) of ref. 1.
HS	W cm ⁻² °C ⁻¹	Gap conductance component through solid-solid contact points when fuel and cladding are in contact. See Eq. (24) of ref. 1.

<u>Name</u>	<u>Unit</u>	<u>Definition</u>
HF	$W\ cm^{-2}\ ^\circ C^{-1}$	Gap conductance component through gas phase between points of contact when fuel-cladding gap is closed. See Eq. (23) of ref. 1.
G1	cm	Temperature jump distance for gas at fuel surface
G2	cm	Temperature jump distance for gas at cladding inner surface
13. COMMON/INP1/		
IDATA ICON ADATA BDATA IBDATA		See Appendix B
14. COMMON/INP2/		
CDATA JDATA DDATA		See Appendix B
15. COMMON/INP3/		
KDATA EDATA FDATA GDATA		See Appendix B
16. COMMON/STORE1/		
SR(I)	psi	Stored radial stress at <i>i</i> th cladding node
ST(I)	psi	Stored tangential stress at <i>i</i> th cladding node
SZ(I)	psi	Stored axial stress at <i>i</i> th cladding node
EPSR(I)		Stored radial plastic strain at <i>i</i> th cladding node
EPST(I)		Stored tangential plastic strain at <i>i</i> th cladding node
RC(I)	cm	Stored radius of <i>i</i> th cladding node

<u>Name</u>	<u>Unit</u>	<u>Definition</u>
17. COMMON/STORE2/		
XSR(I)	psi	New radial stress at <i>i</i> th cladding node
XST(I)	psi	New tangential stress at <i>i</i> th cladding node
XSZ(I)	psi	New axial stress at <i>i</i> th cladding node
XEPSR(I)		New radial plastic strain at <i>i</i> th cladding node
XEPST(I)		New tangential plastic strain at <i>i</i> th cladding node
XRC(I)	cm	New radius of <i>i</i> th cladding node
18. COMMON/STORE3/		
CIR	cm	Cladding inner radius
COR	cm	Cladding outer radius
19. COMMON/HYDRO/		
PH(I)	psi	Hydrostatic stress at <i>i</i> th fuel node
20. COMMON/BURN/		
BU(I)	%	Volume swelling in <i>i</i> th fuel increment at the end of the previous cycle
XBU(I)	%	Current volume swelling in <i>i</i> th fuel increment
BUSAVE(I)	% FIMA	Burnup (fissions per initial heavy metal atom) in the <i>i</i> th fuel increment at the end of the current cycle
XB(I)	%	Volume swelling in <i>i</i> th fuel increments as calculated during the previous iteration of the current cycle
21. COMMON/SIGEPS/		
SIGR(I)	psi	Current radial stress at <i>i</i> th cladding node
SIGT(I)	psi	Current tangential stress at <i>i</i> th cladding node

<u>Name</u>	<u>Unit</u>	<u>Definition</u>
SIGZ(I)	psi	Current axial stress at <i>i</i> th cladding node
EPR(I)		Current radial plastic strain at <i>i</i> th cladding node
EPT(I)		Current tangential plastic strain at <i>i</i> th cladding node
RAD(I)	cm	Current radius of <i>i</i> th cladding node
22. COMMON/CYCLE/		
NCYC		Cycle number
23. COMMON/REDIST/		
RF(I)		Ratio Pu/(U+Pu) at end of cycle in <i>i</i> th fuel increment
24. COMMON/EAMU/		
XE(I)	psi	Elastic modules at <i>i</i> th node
XA(I)	$^{\circ}\text{C}^{-1}$	Coefficient of thermal expansion at <i>i</i> th node
XPU(I)		Poisson's ratio at <i>i</i> th node
25. COMMON/CPUMIN/		
XCPU	min	CPU time used
26. COMMON/AOUT/		
XOUT YOUT ZOUT		Output arrays, where values are set at the end of SUBROUTINE HUB, and can be output from FMODEL at the end of each cycle, at the user's option
27. COMMON/ONE/		
SIGRR	psi	Coolant pressure exerted at outer cladding surface
SIGRI	psi	Pressure exerted on inner cladding surface from fission gas and fuel-cladding contact

<u>Name</u>	<u>Unit</u>	<u>Definition</u>
NOFI		Number of iterations allowed for convergence of iterative mechanical solutions
NOFS		Number of cladding nodes
ACC		Acceleration factor. Not used in this version
NODT		Number of creep time intervals per time period. Not used in this version
DT	hr	Length of a creep time period
HRS	hr	Duration of a cycle
DHRS	hr	Duration of a subcycle
COOL	°C	Coolant temperature
FLUX	neutrons cm ⁻² sec ⁻¹	Neutron flux (energies >0.1 MeV)
28. COMMON/TWO/		
TEMP(I)	°C	Temperature at <i>i</i> th cladding node
E(I)	psi	Elastic modulus at <i>i</i> th cladding node
YMU(I)		Poisson's ratio at <i>i</i> th cladding node
KIND(I)		Not used
29. COMMON/TWOX/		
XALPHA(I)	°C ⁻¹	Coefficient of linear thermal expansion at <i>i</i> th cladding node
30. COMMON/THREE/		
NFUEL		Number of fuel increments
NCLAD		Number of cladding increments
GAMF	W/g	Fuel gamma heating rate
GAMC	W/g	Cladding gamma heating rate
RHOT	g/cm ³	Theoretical density of fuel

<u>Name</u>	<u>Unit</u>	<u>Definition</u>
RHOCJ.D	g/cm ³	Cladding density
XMEV	MeV/fission	Fission energy
31. COMMON/THREEX/		
RHOA		Fabricated fuel density, expressed as a fraction of theoretical density,
32. COMMON/FOUR/		
XHFILM	W cm ⁻² °C ⁻¹	Cladding film conductance
XHGAP	W cm ⁻² °C ⁻¹	Fuel-cladding gap conductance
IPSTD		Control integer, which controls form of equation used for porosity correction of thermal conductivity from that of 100%-dense material 0 Maxwell-Eucken correction 1 Loeb correction
ALPHA		Value of constant used in Loeb correction
BETA		Value of constant used in Maxwell-Eucken correction
ICLAD		Integer designation for the cladding, which controls the thermal conductivity values used in SUBROUTINE KCIAD 1 for type 304 stainless steel 2 for type 316 stainless steel 3 for type 347 stainless steel
33. COMMON/FIVE/		
GPRES	psi	Gas pressure
34. COMMON/SIX/		
ERATE	%/at. % burnup	Swelling rate in fuel due to solid fission products

<u>Name</u>	<u>Unit</u>	<u>Definition</u>
35. COMMON/SEVEN/		
AR(I)	cm ²	Initial (cold) cross sectional area of <i>i</i> th fuel increment
GCM(I)	g/cm	Initial (cold) mass per unit length for fuel in <i>i</i> th increment
FD(I)		Not used
FR(I)		Not used
36. COMMON/EIGHT/		
XEMOL	moles	Moles of xenon present in pin
XKRMOL	moles	Moles of krypton present in pin
FREL		Fraction of fission gas released
37. COMMON/NINE/		
POWFAC		Power factor. This is the fractional power at a given axial node, based on a value of 1 for the peak rod position

REFERENCE

1. C. M. Cox, F. J. Homan, and R. L. Diamond, "Description of Fuel-to-Cladding Gap Conductance," *Fuels and Materials Development Program Quart. Progr. Rep. Mar. 31, 1972, ORNL-TM-3793, pp. 25-38.*

APPENDIX B

INPUT GLOSSARY

The INPUT subroutine reads data into several common area arrays. Each location within those arrays is identified in this appendix. The array location, symbol, units, and definition are given. The symbol given is the variable name, which is assigned and used later in the program. For example, it is NFUEL rather than IDATA(5) that is used in the code to represent the number of radial increments in the fuel material. However, a number that is later assigned to NFUEL is introduced into the program through the IDATA(5) location. Some variables assigned into the input arrays are used directly and are not assigned symbols. A blank symbol space reflects this situation. Also, some input variables are dimensionless and therefore have blank spaces in the units column.

The advantage of this system of input is that all input data can be easily output and checked for accuracy. Also, additional variables can be added to the input without making changes in the INPUT subroutine.

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
IDATA(1)			Number of points to be read into the ADATA array. This number must be 54 or fewer.
(2)			Number of rows in the BDATA array. This corresponds to the number of cycle-dependent real number variables. This number must be ten or fewer.
(3)	NSETS		Number of columns in BDATA array. This corresponds to the number of cycles.
(4)			Number of rows in the IBDATA array. This is the number of cycle-dependent integer variables. This number must be five or fewer.
(5)	NFUEL		Number of fuel radial increments
(6)	NCLAD		Number of cladding radial increments
(7)	NREG		Number of axial regions
(8)	NREL		Number of gas release-temperature pairs

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
IDATA(9)	NPMIN		Number of minimum porosity-temperature pairs
(10)	NOFI		Number of iterations in EPLAS and CREEP. If convergence is not attained in this number of iterations, the calculation proceeds without convergence.
(11)	IK		Controls thermal conductivity function used for the fuel material. When IK is 1 STDFCN is called, when IK is 2 GEFCN is called.
(12)	IPSTD		Controls porosity correction factor used with STDFCN. The convention is the same as discussed in the PROFIL code. ¹
(13)			Not used
(14)	ICLAD		Controls cladding thermal conductivity values used 1 for type 304 stainless steel 2 for type 347 stainless steel 3 for type 316 stainless steel
(15)	NMOD		Number of cladding moduli-temperature pairs to be input
(16)	NCLE		Number of cladding thermal expansion coefficient-temperature pairs to be input
(17)	NYS		Number of cladding yield strength-temperature pairs to be input
(18)	NPROP		Number of property-temperature pairs to be input into the DDATA array
JDATA(1)	IRFUEL		Controls generation of radial nodes in fuel when 1 the radii are input when 2 radii are calculated on an equal thickness basis when 3 radii are calculated on an equal volume basis

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
JDATA(2)	IRCIAD		Controls generation of cladding nodes
(4)	ICON9		Controls path in PLSTR 1 use built-in tensile data for strain-strain analysis 2 use input tensile data
(5)	ICON1		Controls path in PLSTR, XPLSTR, and ALPH 1 annealed cladding 2 20%-cold-worked cladding
(6)	ICON17		Controls use of irradiation-enhanced creep equation 0 irradiation-enhanced creep not considered 1 irradiation-enhanced creep is considered
(7)	ICON21		Controls use of RPP 0 not called 1 called
(8)			Controls degree of axial restraint in FEXP 0 isotropic swelling and thermal expansion 1 complete axial restraint
(9)			Controls input of gap conductance when this quantity is input rather than calculated 0 use constant value 1 input value for each cycle
(10)			The number of the axial region for which detailed output is to be accomplished
(11)	NINS		Number of increments in thermal insulator
(12)	IRINS		Controls insulator radii generation
(13)			Number of data values to be read into EDATA array
(14)			Number of data values to be read into FDATA array
(15)			Number of data values to be read into GDATA array

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
ICON(1)			Controls output from RADIAL
(2)			Controls output from GSM
(3)			Controls output from OUT1
(4)			Controls output from EPLAS (after convergence)
(5)			Controls output from CREEP (after convergence)
(6)			Controls output from EPLAS (after each iteration)
(7)			Controls output from SWELL
(8)			Controls output from FEXP
(9)			Controls output of gap conduct- ance convergence in TDIST
(10)			Controls output of plasticity temperature from PLAST
(11)			Controls use of thermal insulator 0 not used 1 used
(12)			Controls output from MECH
(13)–(14)			Not used
(15)			Controls degree of axial restraint in FEXP
(16)			Controls output in HUB after contact pressure convergence
(17)			Controls DMAX value used in PVEL 0 use $DMAX = (R_{i+1} - R_i)/2$ 1 input DMAX
(18)			Controls creep equation used in XPLSTR 0 WARD 1 Swindeman
(19)			Controls output in GCON
(20)			Controls output from RPP

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
ICON(21)			Controls density correction for insulator thermal conductivity 0 do not correct for density 1 correct for density
(22)			Controls output from PVEL
(23)			Controls gap conductance calcu- lation 0 input HGAP 1 calculate HGAP
(24)			Controls cladding swelling cal- culation 0 constant swelling 1 swelling calculated at each node
(25)–(29)			Not used
(30)			Controls output at end of HUB
(31)			Controls output from iterative steps in CREEP
(32)			Controls output before iterative fuel-cladding contact pressure calculation in HUB
(33)–(39)			Not used
(40)			Controls output from FMODEL at end of each cycle 0 do not print any individual radial calculations 1 print all individual radial calculations 2 print radii only 3 print temperatures only 4 print densities only 5 print radii and temperatures 6 print radii and densities 7 print temperatures and densities
(41)–(54)			Not used

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
ADATA(1)	RCLAD	cm	Cladding outer radius
(2)	THICK	cm	Cladding thickness
(3)	XMEV	MeV/fission	Fission energy
(4)	RVOID	cm	Radius of as-fabricated central void
(5)	XMW	g/mole	Molecular weight of fuel
(6)	RHUT	g/cm ³	Theoretical fuel density
(7)	RHOA		Attained fuel density (fraction of theoretical)
(8)	GAMF	W/g	Gamma heating rate of fuel
(9)	GAMC	W/g	Gamma heating rate of cladding
(10)	RHOCLD	g/cm ³	Cladding density
(11)	XHFILM	W cm ⁻² °C ⁻¹	Heat transfer coefficient of cladding film
(12)	XHGAP	W cm ⁻² °C ⁻¹	Heat transfer coefficient of fuel-cladding gap
(13)	ALPHA		Same as in PROFIL code ¹
(14)	BETA		Same as in PROFIL code ¹
(15)	ERATE	(at. % burnup) ⁻¹	Solid fission product swelling rate
(16)		kW/ft	Normal power heat rate at peak power position
(17)		μm	Initial grain size of fuel
(18)			Initial oxygen-to-metal ratio of fuel
(19)	XFLUX	neutron cm ⁻² sec ⁻¹	Maximum neutron flux (>0.1 MeV)
(20)	FDOT	fissions cm ⁻³ sec ⁻¹	Fission rate at peak normal heat rate
(21)	VPLEN	cm ³	Plenum volume (used in multinode version only)
(22)	FMOLE	moles	Moles of fill gas (multinode version only)

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
ADATA(23)		cm	Length of an axial region (multinode version only)
(24)			Initial Pu/(U+Pu) ratio
(25)		g metal/cm ³	Initial fuel density as heavy metal
(26)		cm ³	Initial fuel volume
(27)			Ratio of Pu fissions to (U+Pu) fissions
(28)		°C	Temperature at which pin is examined
(29)		°C ⁻²	Slope (m) of expression for fuel thermal expansion $\alpha_f = (mT + b) \times 10^{-6} \text{ } ^\circ\text{C}^{-1}$
(30)		psi	Maximum allowable contact pressure used in CONV
(31)		cm	Thickness of thermal insulator
(32)		cm	Gap between cladding and thermal insulator
(33)		W/g	Gamma heating rate for thermal insulator
(34)		g/cm ³	Density of insulator material
(35)		W cm ⁻¹ °C ⁻¹	Intercept (b) in cladding ther- mal conductivity equation $k(T) = mT + b \quad T = ^\circ\text{C}$ $k = \text{W cm}^{-1} \text{ } ^\circ\text{C}^{-1}$
(36)		W cm ⁻¹ °C ⁻²	Slope (m) of cladding thermal conductivity equation (see above)
(37)		W cm ⁻² °C ⁻¹	Heat transfer coefficient across cladding-insulator gap
(38)		°C ⁻¹	Intercept (b) for fuel thermal expansion expression [(see ADATA(29) for equation)]
(39)		°C	Melting temperature of fuel

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
ADATA(40)		$W\ cm^{-1}\ ^\circ C^{-1}$	Value of A in the polynomial expression for the insulator thermal conductivity $k(T) = A + BT + CT^2 + DT^3 + ET^4$
(41)		$W\ cm^{-2}\ ^\circ C^{-2}$	Value of B in above equation
(42)		$W\ cm^{-2}\ ^\circ C^{-3}$	Value of C
(43)		$W\ cm^{-2}\ ^\circ C^{-4}$	Value of D
(44)		$W\ cm^{-2}\ ^\circ C^{-5}$	Value of E
(45)		$W\ cm^{-1}\ ^\circ C^{-1}$	Value of A in the polynomial expression for the fuel thermal conductivity [see ADATA(40) for the equation]. These values do not need to be input if the fuel thermal conductivity is described by some other expression
(46)		$W\ cm^{-2}\ ^\circ C^{-2}$	Value of B in polynomial expansion for fuel thermal conductivity
(47)		$W\ cm^{-2}\ ^\circ C^{-3}$	Value of C
(48)		$W\ cm^{-2}\ ^\circ C^{-4}$	Value of D
(49)		$W\ cm^{-1}\ ^\circ C^{-5}$	Value of E in polynomial expansion for fuel thermal conductivity
(50)		g/cm^3	Theoretical density of thermal insulator
(51)		cm	rms surface roughness of material at cladding inner surface
(52)		cm	rms surface roughness of insulator material at outer surface
(53)		$^\circ C^{-2}$	Slope (m) in equation for insulator thermal expansion $\alpha_i = (mT + b) \times 10^{-6}\ ^\circ C^{-1}$
(54)		$^\circ C^{-1}$	Intercept (b) in above equation for insulator thermal expansion

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
EDATA(1)		cm	Distance a pore can move (used in SUBROUTINE PORE) before temperature is recalculated. Do not need when ICON(17) = 0
(2)		cm	rms surface roughness of material at insulator inner surface
(3)		cm	rms surface roughness of material at fuel outer surface
(4)			Maximum permissible fraction of theoretical density that can be attained by the fuel because of restructuring.
BDATA(1,J)	HRS(J)	hr	Duration of <i>j</i> th cycle
(2,J)	DHRS(J)	hr	Duration of <i>j</i> th subinterval
(3,J)	XDT(J)	hr	Duration of creep interval during <i>j</i> th cycle
(4,J)	PF(J)		Power factor for <i>j</i> th cycle
(5,J)	PII(J)	psi	Fission gas pressure at beginning of <i>j</i> th cycle
(6,J)	PIF(J)	psi	Fission gas pressure at end of <i>j</i> th cycle
(7,J)	POUT(J)	psi	Coolant pressure during <i>j</i> th cycle
(8,J)	COOL(J)	°C	Coolant temperature during <i>j</i> th cycle
IBDATA(2,J)	NSTEPS		Control number to direct exit from HUB number of subintervals plus 2 for 1st cycle number of subintervals plus 1 for other cycles

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
IBDATA(3,J)	IRAMP		Power ramp characteristic of j th cycle 0 power decreases at beginning of cycle 1 power increases at beginning of cycle, and cycle follows a period during which the pin was operated at zero power 2 power increases at beginning of cycle from a lower power condition 3 a rapid cooldown occurs at the beginning of the j th cycle 4 pin cooled to room temperature for examination at beginning of j th cycle, but cooldown is gradual 5 j th cycle is a period of steady-state operation 6 very rapid power increase occurs at beginning of j th cycle, fuel and cladding creep cannot relieve initial contact pressure
CDATA(1,J)	RFUEL(J)	cm	Radius of fuel pellets in j th axial region
(2,J)	COOL(J)	$^{\circ}\text{C}$	Coolant temperature for j th axial region
(3,J)	POUT(J)	psi	Coolant pressure for j th axial region
(4,J)	AXPOS(J)	cm	Axial position of j th axial node (from bottom of pin)
(5,J)			Region/peak power ratio
DDATA(1,J)	EM(J)	psi	Cladding elastic modulus corresponding to j th temperature
(2,J)	SM(J)	psi	Cladding shear modulus corresponding to j th temperature
(3,J)	TMOD(J)	$^{\circ}\text{C}$	j th temperature for moduli
(4,J)	CLE(J)	$^{\circ}\text{C}^{-1}$	Linear thermal expansion coefficient for cladding at j th temperature
(5,J)	TCLE(J)	$^{\circ}\text{C}$	j th temperature for thermal expansion coefficients

<u>Array</u>	<u>Symbol</u>	<u>Unit</u>	<u>Definition</u>
DDATA(5,J)	YS(J)	psi	Cladding yield strength corresponding to <i>j</i> th temperature
(7,J)	TYS(J)	°C	<i>j</i> th temperature for yield strengths
(8,J)	FREL(J)		Fission gas release fraction corresponding to <i>j</i> th temperature
(9,J)	TREL(J)	°C	<i>j</i> th temperature for fission gas release fractions
(10,J)	XPMIN(J)		Minimum porosity value corresponding to <i>j</i> th temperature
(11,J)	TPMIN(J)	°C	<i>j</i> th temperature for minimum porosity values

REFERENCE

1. C. M. Cox and F. J. Homan, *PROFIL - A One-Dimensional FORTRAN IV Program for Computing Steady-State Temperature Distributions in Cylindrical Ceramic Fuels*, ORNL-TM-2443 (March 1969) and Addendum (August 1969).

APPENDIX C

DETAILS OF FUEL RESTRUCTURING MODEL

It is well known that ceramic fuels restructure during irradiation at elevated temperatures, with the fabricated porosity moving up the temperature gradient toward the thermal center. The restructuring is described in some models by assuming temperature-density pairs and calculating the size of the central void and columnar and equiaxed grain regions on a mass balance basis. For instance, it would be assumed that all the fuel above some critical temperature T_e would form equiaxed grains of density D_e , and all fuel above some higher temperature T_c would form columnar grains of density D_c , where $D_c > D_e$. The PROFIL code¹ uses this empirical approach. Although this technique is useful for some applications, it is clearly limited by its inability to consider the time-dependent aspects of fuel restructuring. Time dependence is important in modeling fuel-cladding mechanical interaction because of differential thermal expansion of fuel and cladding during startup or power increases. During initial startup the fuel has not restructured; therefore fuel temperatures are higher than they will be later in life at the same heat rate. Higher fuel temperatures mean more fuel thermal expansion and higher contact pressures between the fuel and cladding. As restructuring proceeds the fuel gradually becomes more dense, increasing its thermal conductivity. This causes fuel temperatures at constant heat rate to gradually decrease, diminishing the fuel-cladding mechanical interaction. When using the empirical model with the temperature-density pairs, one is faced with the choice of modeling the mechanical interaction on the basis of fully restructured fuel and underestimating the mechanical interaction, or on the basis of nonrestructured fuel and overestimating it.

The time-dependent fuel restructuring model employed in FMODEL is based on Nichols'² equation for pore velocity:

$$V \approx \frac{9P_0\Omega \Delta H_v \left[N (M_1 + M_2) \right]^{1/2} \exp \left(\frac{-\Delta H_v^*}{RT} \right) \frac{dT}{dx}}{16P_0^2 T^{3/2} (2\pi k M_1 M_2)^{1/2}} \quad (C1)$$

where

P_0 = a constant (dyne/cm²),

Ω = fuel molecular volume (cm³/molecule),

ΔH_v = molar heat of vaporization (erg/mole),

ΔH_v^* = molar heat of vaporization (cal/mole),

P = total pressure in pore (dyne/cm²),

$N = R/k$ = Avogadro's number (atoms/mole),

k = boltzmann constant = 1.38047×10^{-16} erg/°K,

R = gas constant = 1.986 cal/mole⁻¹ °K⁻¹

dT/dx = temperature gradient (°C/cm),

M_1 = molecular weight of fuel (g/mole),

M_2 = molecular weight of primary vapor constituent (g/mole), and

$\pi\sigma^2$ = cross section for collisions between fuel and vapor species (cm²).

It should be noted that the pore velocity as given in Eq. (C1) is independent of pore size and shape. According to this equation all pores at a given position within the fuel will move with the same velocity. To make use of Eq. (C1) within the framework of the FMODEL code, several assumptions are required. In FMODEL the fuel is divided into a user-specified number of radial increments. The temperatures and temperature gradients are computed at each of $n + 1$ radial nodes, where n is the number of increments. The initial fuel density is assumed to be constant, and subsequent densities are constant for any given increment. The densities of adjacent increments may be higher or lower, but there is no variation from one node to the next. This is equivalent to a density step variation with radial position. Temperatures and temperature gradients are assumed to vary linearly from node to node. Knowing the temperature, temperature gradient, and gas pressure in the pore at each node, the pore velocity at each node can be calculated with Eq. (C1). It is assumed that a pore moves with a velocity calculated at a given node throughout the "neighborhood" of the node. Time periods are selected so that no pore can move further than one-third of the increment thickness; this defines the maximum "neighborhood" for this assumption. Finally, it is assumed that initially the axial section of fuel under study contains N pores, each having a volume V .

To describe mathematically the restructuring that occurs in each fuel increment during a time period of t sec, certain symbols must be defined. They are

N = the number of pores present in the axial section of fuel at time = 0,

V = the volume of a single pore,

A_i = the cross sectional area of the i th radial increment,

R_i = the inner radius of the i th radial increment,

v_i = the velocity of a pore at R_i ,

t = the time period being considered (sec),

N_i = the number of pores in the i th increment at the beginning of the time period,

N_i' = the number of pores that leave the i th increment during the time period,

N_{i+1}' = the number of pores that enter the i th increment (or leave the $i+1$ increment) during the time period,

N_i'' = the number of pores in the i th increment at the end of the time period,

P_i = the porosity of the i th increment at the end of the time period, and

$(P_i)_0$ = the porosity of the i th increment at the beginning of the time period.

In t sec, all pores in the annulus bounded by R_i and $R_i + v_i t$ will leave the i th increment, and all pores in the annulus bounded by R_{i+1} and $R_{i+1} + v_{i+1} t$ will enter. Therefore

$$N_i' = \frac{N_i \pi}{A_i} \left[(R_i + v_i t)^2 - R_i^2 \right], \quad (C2)$$

$$N_{i+1}' = \frac{N_{i+1} \pi}{A_{i+1}} \left[(R_{i+1} + v_{i+1} t)^2 - R_{i+1}^2 \right], \quad (C3)$$

and

$$N_i'' = N_i + N_{i+1}' - N_i'. \quad (C4)$$

The fractional porosity in any radial increment is given by the pore volume divided by the total volume, or for a unit axial length, the initial and final porosity values for the i th increment for any time period are given as

$$(P_i)_0 = N_i V / A_i , \quad (C5)$$

and

$$P_i = \tilde{N}_i V / A_i . \quad (C6)$$

Thus, the ratio of porosities can be expressed as

$$P_i / (P_i)_0 = \tilde{N}_i / N_i . \quad (C7)$$

Substituting Eqs. (C2), (C3), and (C4) into (C7), the ratio becomes

$$\begin{aligned} \frac{P_i}{(P_i)_0} = 1 + \frac{\pi \tilde{N}_{i+1}}{N_i A_{i+1}} \left[(R_{i+1} + V_{i+1} t)^2 - R_{i+1}^2 \right] \\ - \frac{\pi}{A_i} \left[(R_i + V_i t)^2 - R_i^2 \right] . \end{aligned} \quad (C8)$$

From (C5)

$$N_i = (P_i)_0 A_i / V , \text{ and}$$

$$N_{i+1} = (P_{i+1})_0 A_{i+1} / V .$$

Thus the porosity ratio reduces to

$$\frac{P_i}{(P_i)_0} = 1 + \frac{\pi (P_{i+1})_0}{(P_i)_0 A_i} \left[(R_{i+1} + V_{i+1} t)^2 - R_{i+1}^2 \right] - \frac{\pi}{A_i} \left[(R_i + V_i t)^2 - R_i^2 \right] . \quad (C9)$$

At time zero the ratio $(P_{i+1})_0 / (P_i)_0$ is unity. At any other time, values of $(P_i)_0$ and $(P_{i+1})_0$ are both known from previous application

of Eq. (C9). Therefore, the amount of restructuring in the i th increment can be expressed in terms of bubble velocities, geometry, and the length of time considered. The number of pores (N) and the volume of a single pore (V) have cancelled out of the expression.

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APPENDIX D

DETAILS OF THE FUEL-CLADDING MECHANICAL INTERACTION MODEL

Two causes of mechanical interaction between fuel and cladding are considered in FMODEL; differential thermal expansion between fuel and cladding during power increases, and fuel swelling during periods of steady-state operation. The fuel cracking model outlined in Appendix F (see PLAST) is important in both cases.

At low heat rates, where the rupture modulus of the fuel is not exceeded, the change in geometry of the fuel pellet is calculated in the same manner as for the cladding. The details of this calculation are presented in Appendix E. At moderate and high heat rates the fuel is assumed to crack, as outlined in Appendix F. The formation of the cracks relieves the thermal stresses in the fuel pellet, and each radial increment of fuel expands thermally in accordance with its average temperature and thermal expansion coefficient.

During power changes the time rate of change of linear heat rate is assumed constant. The duration of a power ramp is divided into a number of time steps Δt . The length of the time steps is under the control of the user. During each Δt the heat rate of the pin will change by ΔQ . Thermal expansion will cause changes in the outer fuel diameter (ΔD_f) and the cladding inner diameter (ΔD_c). The size of the new fuel-cladding diametral gap is given by

$$\Delta = G_0 + \Delta D_c - \Delta D_f, \quad (D1)$$

where G_0 is the size of the gap at the beginning of the time step. If the calculated gap size (Δ) after a power change is negative, the fuel-cladding gap has closed because of differential thermal expansion, and mechanical contact exists between the fuel and cladding. The heat rate at which the gap size becomes zero is determined by linear interpolation between the existing value of Δ and the value calculated after the previous power change. The position of the radial nodes in the fuel are "frozen" at this point so that the effect of further increases in power on the geometry of the pellet can be determined. It is assumed that the hot plastic fuel interior to the cracked region cannot expand thermally

in the radial direction after the gap has closed. The contact pressure at the fuel-cladding interface, which is transferred to the outer boundary of the hot plastic fuel core by the cracked fuel region, forces all thermal expansion in this hot core into the axial direction. The value of ΔD_f due to further power increases after gap closure is due only to the thermal expansion calculated for the fuel in the cool cracked region.

To calculate the magnitude of the contact pressure between fuel and cladding during a time period Δt after gap closure, an iterative scheme is used whereby the existing contact pressure at the beginning of the time step (this will be fission gas pressure if the gap was open at the beginning of the time step) is repeatedly doubled until the correct contact pressure range is bracketed. Then the bracket is repeatedly halved until the contact pressure is within 1% of the previously calculated value. The basis of the iteration is the amount of change in the cladding inner diameter and fuel outer diameter due to creep in response to the contact pressure. During a period of time Δt the cladding inner diameter will increase by an amount Δ_c in response to the pressure. During the same period of time the fuel outer diameter will decrease by an amount Δ_f due to the pressure transmitted from the fuel-cladding interface to the surface of the hot plastic core by the cracked outer region of fuel. Thus when the relation

$$\Delta_c + \Delta_f = -\Delta, \quad (D2)$$

is satisfied, the contact pressure used to calculate Δ_c and Δ_f represents the average contact pressure during the time step.

Calculation of the contact pressure due to fuel swelling is similar to what has already been described for differential thermal expansion. The same assumption regarding the hot plastic core is used. All swelling in this region is assumed to occur in the axial direction after the fuel-cladding gap has closed, whereas the cool cracked fuel region swells isotropically. During a period of time Δt the volume change in the cool cracked fuel region will be calculated in SWELL, and each radial fuel increment will have a value of $\Delta V/V$. The total amount of swelling

in the cracked region therefore

$$\left(\frac{\Delta V}{V}\right)_{NP} = \sum_{i=I_P}^N \frac{\left(\frac{\Delta V}{V}\right)_i V_i}{V_{NP}}, \quad (D3)$$

where

$(\Delta V/V)_{NP}$ = fraction volume swelling in nonplastic fuel region,

N = number of radial fuel increments,

I_P = number of first nonplastic fuel increment,

$(\Delta V/V)_i$ = fractional volume swelling in the i th fuel increment,

V_i = initial volume of the i th fuel increment, and

V_{NP} = initial volume of nonplastic fuel.

Now,

$$\left(\frac{\Delta V}{V}\right)_{NP} = \frac{V_t - V_{NP}}{V_{NP}} = \frac{V_t}{V_{NP}} - 1,$$

where

V_t = the volume of nonplastic fuel at the time of the calculation,
and

$$\frac{V_t}{V_{NP}} = \frac{\pi(h + \Delta h) \left[(R_o + \Delta R_c)^2 - (R_c + \Delta R_c)^2 \right]}{\pi h (R_o^2 - R_c^2)}, \quad (D5)$$

R_o = the pellet radius, or outer radius of the cracked fuel, and

R_c = the crack radius, or inner radius of the cracked fuel.

By eliminating the $(\Delta R)^2$ and $\Delta h \Delta R$ terms, Eq. (D5) reduces to

$$\frac{V_t}{V_{NP}} = \frac{R_o^2 + 2R_o \Delta R_o - R_c^2 - 2R_c \Delta R_c}{R_o^2 - R_c^2} + \frac{\Delta h}{h}. \quad (D6)$$

Now, from the isotropic assumption,

$$\Delta R_o / R_o = \Delta R_c / R_c = \Delta h / h = \delta ,$$

we obtain

$$2R_o \Delta R_o = 2R_o^2 \delta ,$$

$$2R_c \Delta R_c = 2R_c^2 \delta ,$$

$$\frac{V_t}{V_{NP}} = \frac{R_o^2 - R_c^2 + 2\delta(R_o^2 - R_c^2)}{R_o^2 - R_c^2} + \delta . \quad (D7)$$

$$V_t / V_{NP} = 1 + 3\delta ,$$

$$\Delta R_o / R_o = (\Delta V / V)_{NP} / 3 . \quad (D8)$$

Thus, knowing R_o and the fractional volume swelling in each nonplastic fuel increment during the time period Δt , we can calculate the change in the pellet radius ΔR_o . This value is then used on the right side of Eq. (D2) to determine the contact pressure.

For mechanical interaction due to both differential thermal expansion and fuel swelling, pressure is transmitted from the fuel-cladding interface to the plastic fuel core by the cool, cracked nonplastic fuel region. Therefore, a change in the outer pellet radius ΔR_o is related to a change in the radius of the plastic core ΔR_c by the following expression

$$\pi h [R_o^2 - (R_o - \Delta R_c)^2] = \pi h [R_c^2 - (R_c^2 - \Delta R_c^2)] .$$

Expanding the terms in parentheses and eliminating the ΔR_o^2 and ΔR_c^2 terms yields

$$\Delta R_o = R_c \Delta R_c / R_o ,$$

where

$$\Delta R_c = \dot{\epsilon}_f R_c \Delta t,$$

$\dot{\epsilon}_f$ = the creep rate of the fuel at the root of the crack.

APPENDIX E

DETAILED DERIVATION OF FINITE DIFFERENCE SOLUTION

List of Symbols

- α linear coefficient of thermal expansion
 a inner radius of cylinder
 A creep equation constant
 b outer radius of cylinder
 B creep equation constant
 E elastic modulus
 ϵ_r total radius strain
 ϵ_θ total tangential strain
 ϵ_z total axial strain
 ϵ_r^P plastic radial strain = $\frac{\epsilon_P}{3\epsilon_{et}} (2\epsilon_r - \epsilon_\theta - \epsilon_z)$
 ϵ_θ^P plastic tangential strain = $\frac{\epsilon_P}{3\epsilon_{et}} (2\epsilon_\theta - \epsilon_r - \epsilon_z)$
 ϵ_z^P plastic axial strain = $-(\epsilon_r^P + \epsilon_\theta^P)$
 ϵ_{et} equivalent total strain =

$$\frac{\sqrt{2}}{3} \left[(\epsilon_r - \epsilon_\theta)^2 + (\epsilon_\theta - \epsilon_z)^2 + (\epsilon_r - \epsilon_z)^2 \right]^{1/2}$$

 ϵ_P equivalent plastic strain =

$$\frac{\sqrt{2}}{3} \left[(\epsilon_r^P - \epsilon_\theta^P)^2 + (\epsilon_\theta^P - \epsilon_z^P)^2 + (\epsilon_r^P - \epsilon_z^P)^2 \right]^{1/2}$$

 $\Delta\epsilon_r^C$ radial creep strain increment during time interval Δt =

$$\frac{\Delta\epsilon_{ec}}{2\sigma_e} (2\sigma_r - \sigma_\theta - \sigma_z)$$

 $\Delta\epsilon_\theta^C$ tangential creep strain increment during time interval Δt =

$$\frac{\Delta\epsilon_{ec}}{2\sigma_e} (2\sigma_\theta - \sigma_r - \sigma_z)$$

- $\Delta \epsilon_{ec}$ creep strain during time interval $\Delta t = \dot{\epsilon} \Delta t$
 μ Poisson's ratio
 n creep equation constant
 N number of radial nodes
 P_i internal pressure
 P_o external pressure
 Q creep equation constant (activation energy)
 R universal gas constant
 σ_r radial stress
 σ_θ tangential stress
 σ_z axial stress
 σ_e equivalent stress =

$$\frac{1}{2} \left[(\sigma_r - \sigma_\epsilon)^2 + (\sigma_\theta - \sigma_z)^2 + (\sigma_r - \sigma_z)^2 \right]^{1/2}$$

- T temperature
 T_a absolute temperature
 Δt length of time interval

Basic Equations

The assumptions associated with the finite difference solution for fuel pin cladding include axial symmetry, generalized plane strain,* and validity of the deformation theory of plasticity. Under these circumstances the equilibrium equation can be written¹

$$\frac{d\sigma_r}{dr} + \frac{\sigma_r - \sigma_\theta}{r} = 0, \quad (E1)$$

and the compatibility equation is¹

$$\frac{d\epsilon_\theta}{dr} + \frac{\epsilon_\theta - \epsilon_r}{r} = 0. \quad (E2)$$

*A plane perpendicular to the cladding axis remains plane after deformation, or $\epsilon_z = \text{constant}$.

Since boundary conditions are usually described in terms of stresses, it is convenient to solve mechanics problems in terms of stresses and then calculate the strains due to these stresses. The stress-strain relationships are given below.²

$$\epsilon_r = \frac{1}{E} [\sigma_r - \mu(\sigma_\theta + \sigma_z)] + \alpha T + \epsilon_r^P, \quad (E3)$$

$$\epsilon_\theta = \frac{1}{E} [\sigma_\theta - \mu(\sigma_r + \sigma_z)] + \alpha T + \epsilon_\theta^P, \quad (E4)$$

$$\epsilon_z = \frac{1}{E} [\sigma_z - \mu(\sigma_r + \sigma_\theta)] + \alpha T + \epsilon_z^P. \quad (E5)$$

Substitution of Eqs. (E3) and (E4) into the compatibility Eq. (E2) yields

$$\frac{d}{dr} \left[\frac{\sigma_\theta}{E} - \frac{\mu}{E}(\sigma_r + \sigma_z) + \alpha T + \epsilon_\theta^P \right] + \frac{1}{r} \left[\frac{1+\mu}{E}(\sigma_\theta - \sigma_r) + \epsilon_\theta^P - \epsilon_r^P \right] = 0. \quad (E6)$$

If Eq. (E5) is solved for σ_z and the result substituted into Eq. (E6), after collecting terms we have

$$\begin{aligned} \frac{d}{dr} \left[\frac{\sigma_\theta - \mu\sigma_r}{E} - \mu\epsilon_z + \alpha T(\mu + 1) + \mu\epsilon_z^P - \frac{\mu^2}{E}(\sigma_\theta + \sigma_r) + \epsilon_\theta^P \right] = \\ \frac{1+\mu}{Er}(\sigma_r - \sigma_\theta) + \frac{\epsilon_r^P - \epsilon_\theta^P}{r}. \end{aligned} \quad (E7)$$

From the plane strain assumption,

$$\epsilon_z = \text{constant},$$

$$\frac{d}{dr}(-\mu\epsilon_z) = 0.$$

In addition, it is assumed that no volume change accompanies plastic flow. Therefore ϵ_z^P can be expressed³ in terms of ϵ_r^P and ϵ_θ^P :

$$\epsilon_r^P + \epsilon_\theta^P + \epsilon_z^P = 0 . \quad (E8)$$

Equation (E7) can now be restated

$$\frac{d}{dr} \left[\frac{\sigma_\theta - \mu \sigma_r}{E} + (\mu + 1) \alpha T - \mu (\epsilon_\theta^P + \epsilon_r^P) - \frac{\mu^2}{E} (\sigma_r + \sigma_\theta) + \epsilon_\theta^P \right] =$$

$$\frac{1 + \mu}{E} (\sigma_r - \sigma_\theta) + \frac{\epsilon_r^P - \epsilon_\theta^P}{r} . \quad (E9)$$

Equations (E1) and (E9) now represent a pair of simultaneous differential equations involving only σ_θ , σ_r , ϵ_θ^P , and ϵ_r^P . If the cylinder is not stressed past its elastic limit ϵ_θ^P and ϵ_r^P are zero and two equations with two unknowns can be solved for the radial and tangential stresses. If the elastic limit is exceeded an iterative solution is used, whereby ϵ_θ^P and ϵ_r^P are estimated from the stress level calculated in the previous iteration. The estimates are used in Eqs. (E1) and (E9) and new stresses calculated. The process is continued until convergence is achieved.

In an operating fuel pin the cladding is exposed to a severe radial temperature gradient, causing variation in elastic modulus, Poisson's ratio, and linear expansion coefficient with radial position. To deal with this physical situation the finite difference formulation² has been chosen to reduce the differential equations (E1) and (E9) to algebraic form for solution by a standard matrix technique. To apply this method the cylinder is divided into N concentric radial increments having $N + 1$ mesh points or nodes. Then at the midpoint of the i th increment⁴

$$\frac{d\sigma}{dr} = \frac{\sigma_{i+1} - \sigma_i}{r_{i+1} - r_i} , \quad (E10)$$

$$\sigma = (\sigma_{i+1} - \sigma_i)/2 . \quad (E11)$$

Applying Eqs. (E10) and (E11) to Eqs. (E1) and (E9), we have

$$C_i \sigma_{r,i} - D_i \sigma_{\theta,i} - F_i \sigma_{r,i-1} - G_i \sigma_{\theta,i-1} = 0, \quad (\text{E12})$$

$$C'_i \sigma_{r,i} + D'_i \sigma_{\theta,i} - F'_i \sigma_{r,i-1} - G'_i \sigma_{\theta,i-1} = H'_i + P'_i, \quad (\text{E13})$$

where

$$h_i = r_i - r_{i-1} - 1,$$

$$C_i = \frac{1}{h_i} + \frac{1}{2r_i},$$

$$C'_i = \frac{-\mu}{h_i E_i} - \frac{\mu^2}{h_i E_i} - \frac{1+\mu}{2E_i r_i},$$

$$D_i = \frac{1}{2r_i},$$

$$D'_i = \frac{1}{h_i E_i} - \frac{\mu^2}{h_i E_i} + \frac{1+\mu}{2E_i r_i},$$

$$F_i = \frac{1}{h_i} - \frac{1}{2r_{i-1}},$$

$$F'_i = -\frac{\mu}{h_i E_{i-1}} - \frac{\mu^2}{h_i E_{i-1}} + \frac{1+\mu}{2E_{i-1} r_{i-1}},$$

$$G_i = \frac{1}{2r_{i-1}},$$

$$G'_i = \frac{1}{h_i E_{i-1}} - \frac{\mu^2}{h_i E_{i-1}} - \frac{1+\mu}{2E_{i-1} r_{i-1}},$$

$$H'_i = -\frac{1+\mu}{h_i} \left[(\alpha T)_i - (\alpha T)_{i-1} \right],$$

$$X \equiv \begin{bmatrix} \sigma_{r,1} \\ \sigma_{\theta,1} \\ \sigma_{r,2} \\ \sigma_{\theta,2} \\ \sigma_{r,3} \\ \sigma_{\theta,3} \\ \sigma_{r,4} \\ \sigma_{\theta,4} \\ \sigma_{r,5} \\ \sigma_{\theta,5} \end{bmatrix} \quad R \equiv \begin{bmatrix} -P_i \\ H_2' + P_2' \\ 0 \\ H_3' + P_3' \\ 0 \\ H_4' + P_4' \\ 0 \\ H_5' + P_5' \\ 0 \\ -P_o \end{bmatrix}$$

Once σ_r and σ_θ are known at each node, σ_z is calculated by means of the plane strain assumption. For a hollow cylinder with internal pressure P_i , equating forces yields

$$\int_a^b \sigma_z 2\pi r \, dr = \pi a^2 P_i . \quad (E15)$$

From Eq. (E5) we have

$$\sigma_z = E \left[\epsilon_z + \mu(\sigma_r + \sigma_\theta) \right] - \alpha T - \epsilon_z^P , \quad (E16)$$

or

$$\int_a^b E \left[\epsilon_z + \mu(\sigma_r + \sigma_\theta) - \alpha T - \epsilon_z^P \right] r \, dr = \frac{a^2 P_i}{2} . \quad (E17)$$

Now, since $\epsilon_z = \text{constant}$ (from the plane strain assumption),

$$\int_a^b E \epsilon_z r \, dr = \epsilon_z \int_a^b E r \, dr ,$$

$$\epsilon_z = \frac{\frac{\alpha^2 P_i}{2} - \int_a^b E \left[\mu(\sigma_r + \sigma_\theta) - \alpha T - \epsilon_r^z \right] r \, dr}{\int_a^b E r \, dr} . \quad (E18)$$

One evaluates ϵ_z from Eq. (E18) and calculates σ_z from Eq. (E16).

As indicated earlier, Eqs. (E1) and (E9) represent a pair of differential equations with σ_θ , σ_r , ϵ_θ^P , and ϵ_r^P as the variables. From the differential equations a system of $2(N+1)$ algebraic equations have been established by the finite difference technique. The Von Mises yield criterion⁵ is used as a basis to determine if the first calculated stress state is sufficient to cause plastic deformation. To estimate the amount of plastic deformation from the stresses calculated the three assumptions associated with the deformation theory of plasticity are applied.⁴ The first assumption has already been stated as Eq. (E8) — that the volume remains constant during plastic deformation. The other two assumptions, that the directions of principal strains coincide with the directions of principal stresses and the ratio of principal shear strains is equal to the ratio of principal shear stresses, are stated mathematically in Eq. (E19).

$$\frac{\epsilon_r - \epsilon_\theta}{\sigma_r - \sigma_\theta} = \frac{\epsilon_r - \epsilon_z}{\sigma_r - \sigma_z} = \frac{\epsilon_\theta - \epsilon_z}{\sigma_\theta - \sigma_z} = K . \quad (E19)$$

Substitution of Eqs. (E3), (E4), and (E5) into Eq. (E19) yields

$$\frac{\epsilon_r^P - \epsilon_\theta^P}{\sigma_r - \sigma_\theta} = \frac{\epsilon_r^P - \epsilon_z^P}{\sigma_r - \sigma_z} = \frac{\epsilon_\theta^P - \epsilon_z^P}{\sigma_\theta - \sigma_z} = K - \frac{1 + \mu}{E} . \quad (E20)$$

Three new quantities are now defined:⁶

1. Equivalent stress

$$\sigma_e = \frac{1}{2} \left[(\sigma_r - \sigma_\theta)^2 + (\sigma_\theta - \sigma_z)^2 + (\sigma_r - \sigma_z)^2 \right]^{1/2} . \quad (E21)$$

2. Equivalent total strain

$$\epsilon_{et} = \frac{\sqrt{2}}{3} \left[(\epsilon_r - \epsilon_\theta)^2 + (\epsilon_\theta - \epsilon_z)^2 + (\epsilon_r - \epsilon_z)^2 \right]^{1/2}, \quad (E22)$$

3. Equivalent plastic strain

$$\epsilon_P = \frac{\sqrt{2}}{3} \left[(\epsilon_r^P - \epsilon_\theta^P)^2 + (\epsilon_\theta^P - \epsilon_z^P)^2 + (\epsilon_r^P - \epsilon_z^P)^2 \right]^{1/2}. \quad (E23)$$

Squaring each term in Eqs. (E19) and (E20) shows that

$$K^2 = 9\epsilon_{et}^2 / 4\sigma_e^2$$

$$\left(K - \frac{1+\mu}{E}\right)^2 = \frac{9}{4} \frac{\epsilon_P^2}{\sigma_e^2}.$$

Therefore,

$$\epsilon_P = \epsilon_{et} - \frac{2}{3} \left(\frac{1+\mu}{E} \right) \sigma_e. \quad (E24)$$

Equation (E24) provides the necessary relation between stress level and plastic deformation needed to estimate ϵ_θ^P and ϵ_r^P . The strain-strain approach is used because of its strongly convergent characteristics.

With this method uniaxial tensile data are used to generate a curve of ϵ_P vs ϵ_{et} through application of Eq. (E24). Figures E-1 and E-2 demonstrate the derivation of a strain-strain curve for annealed and 20%-cold-worked type 316 stainless steel at 400 and 600°C. Once a value for ϵ_P is obtained, values for ϵ_r^P , ϵ_θ^P , and ϵ_z^P are calculated from the following relationships:⁷

$$\epsilon_r^P = \frac{\epsilon_P}{3\epsilon_{et}} (2\epsilon_r - \epsilon_\theta - \epsilon_z), \quad (E25)$$

$$\epsilon_\theta^P = \frac{\epsilon_P}{3\epsilon_{et}} (2\epsilon_\theta - \epsilon_r - \epsilon_z), \quad (E26)$$

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Fig. E-1. Stress versus strain for 20%-cold-worked and annealed type 316 stainless steel.

Fig. E-2. Strain-strain curve for type 316 stainless steel.

$$\begin{aligned}\epsilon_z^P &= \frac{\epsilon_P}{3\epsilon_{et}}(2\epsilon_z - \epsilon_\theta - \epsilon_r) \\ &= -(\epsilon_r^P + \epsilon_\theta^P) .\end{aligned}\tag{E27}$$

Equations (E25) through (E27) provide the necessary values of ϵ_r^P and ϵ_θ^P for use in Eqs. (E12) and (E13) to begin the next iteration. Figure E-3 is a block diagram summarizing the calculation to obtain the stress-strain states on loading.

Fig. E-3. Flow diagram outlining calculational procedure for elastic-plastic solution on loading.

Creep Solution

The combination of stresses calculated in the elastic-plastic solution and elevated temperatures may be sufficient to cause creep in the cladding. To calculate the amount of creep and resulting changes in the stress-strain state at each node, ϵ_r^P and ϵ_θ^P are replaced by $(\epsilon_r^P)'$ and $(\epsilon_\theta^P)'$ in the equations presented in the previous section. The new plastic strains are defined below:

$$(\epsilon_r^P)' = \epsilon_r^P + \Delta\epsilon_r^C, \quad (E28)$$

$$(\epsilon_\theta^P)' = \epsilon_\theta^P + \Delta\epsilon_\theta^C. \quad (E29)$$

Values for $\Delta\epsilon_r^C$ and $\Delta\epsilon_\theta^C$ are derived from the creep law used and the Prandtl-Reuss equations.⁸ Any form of creep law can be used, for example

$$\dot{\epsilon} = A \exp(-Q/RT) \sinh(B\sigma_e/T_a)^n. \quad (E30)$$

$$\Delta\epsilon_C = \dot{\epsilon} \Delta t, \quad (E31)$$

$$\Delta\epsilon_r^C = \frac{\Delta\epsilon_C}{2\sigma_e} (2\sigma_r - \sigma_\theta - \sigma_z), \quad (E32)$$

$$\Delta\epsilon_\theta^C = \frac{\Delta\epsilon_C}{2\sigma} (2\sigma_\theta - \sigma_r - \sigma_z). \quad (E33)$$

Figure E-4 summarizes the steps in the creep solution.

The basic EPLAS and CREEP subroutines are based on computer codes written by Puthoff,⁹ although substantial changes were made in these codes. The method of solving the simultaneous equations was changed, and also some changes in the time schemes were necessary to be compatible with other subroutines in FMODEL.

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Fig. E-4. Flow diagram outlining calculational procedures for creep solution.

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APPENDIX F

DESCRIPTIONS OF INDIVIDUAL SUBROUTINES

ALPH computes cladding swelling due to void formation from fast neutron exposure. It is called from EPLAS and CREEP. Cladding swelling influences the cladding mechanical analysis (described in Appendix E) through the thermal expansion coefficient. Cladding swelling is considered to be analogous to thermal expansion, and an effective thermal expansion coefficient is defined by the following relationship:

$$\alpha = \alpha_T + \% \Delta V/V / 300 T , \quad (F1)$$

where

α = the effective coefficient of linear thermal expansion,

α_T = the coefficient of thermal expansion for the cladding material at the temperature of interest without consideration of the cladding swelling effect,

$\% \Delta V/V$ = the volume percent swelling that has occurred in the cladding at the time of interest, and

T = the temperature of the cladding node being considered.

The cladding swelling in $\% \Delta V/V$ is calculated in the current version of FMODEL from the most recent swelling correlations.¹ The correlation for annealed type 316 stainless steel cladding is given in Eq. (F2), and that for the 20%-cold-worked material in Eq. (F3).

$$\% \Delta V/V = (\phi t)^{f_1(T)} f_2(T) \exp[f_3(T)] , \quad (F2)$$

where

$$f_1(T) = 2.05 - 27/\theta + 78/\theta^2 ,$$

$$\theta = T - 623 ,$$

$$T = ^\circ K ,$$

$$f_2(T) = (T - 40) \times 10^{-10} ,$$

$$f_3(T) = -0.015 T - 5100/T + 32.6 , \text{ and}$$

$$\phi t = \text{fast neutron fluence } (>0.1 \text{ MeV}) .$$

$$\% \Delta V/V = A(\phi t)^{1.5} f_4(T) , \quad (F3)$$

where

$$f_4(T) = 4.028 - 3.712 \times 10^{-2} T + 1.0145 \times 10^{-4} T^2 - 7.879 \times 10^{-3} T^3,$$

$$T = ^\circ\text{C}.$$

Provision is made in ALPH for changes in cladding temperature during the irradiation. Since cladding swelling is calculated on very small time periods, corresponding to the creep intervals from CREEP, power changes, or changes in the fuel pin environment can cause cladding temperatures to change significantly during the irradiation lifetime. The manner in which this is handled in FMODEL is demonstrated in Fig. F-1. Consider one radial cladding node, which begins life at 400°C and operates at that temperature to a fast fluence of 7×10^{22} neutrons/cm². Then a power change brings the temperature of that node to 450°C, where it operates to 9×10^{22} neutrons/cm² fast fluence. At this point the pin is relocated so that the temperature of the node is 700°C, where it operated to 1.2×10^{23} neutrons/cm² fast fluence. Finally, the pin is returned to its original position and power and the irradiation terminated at 1.5×10^{23} neutrons/cm² fast fluence. The calculated cladding swelling would then be $Y_1 + (Y_3 - Y_2) + (Y_5 - Y_4) + (Y_7 - Y_6)$.

When ALPH is called from CREEP, additions are made to the previously calculated $\% \Delta V/V$ value for each cladding node, based on the current node temperature and fluence accumulated during the current creep interval. A new effective thermal expansion coefficient is calculated from Eq. (F1). However, when ALPH is called from EPLAS, no additional swelling increment is calculated, and the effective thermal expansion coefficient is calculated directly from the existing swelling value.

CONV controls the convergence of the fuel-cladding mechanical interaction solution. The thermal expansion of the Fuel (FEXP) and cladding (EPLAS) are calculated at a given level of power. If the outer diameter of an unrestrained fuel exceeds the inner diameter of the cladding, mechanical contact is assumed to occur. To calculate the magnitude of the contact pressure between the fuel and cladding during a small period of time, Δt , an iterative scheme is employed where the basis of the iteration is the contact pressure itself. The existing value of contact pressure is first doubled. The existing value will be fission gas pressure if

Fig. F-1. Metal swelling as influenced by fast neutron fluence and temperature for annealed type 300 stainless steel.

there has been no previous interaction or if the fuel-cladding gap has closed and then opened again. If fuel and cladding were previously in contact (as during a further increase in power after the gap has closed) the existing contact pressure is what the code had previously calculated using the iterative scheme being described here. After the existing value of contact pressure has been doubled, the resulting changes in the cladding inner diameter, Δ_c , and fuel outer diameter, Δ_f , due to the presence of the contact pressure are calculated. A cracked fuel model is used in this calculation, and this is described in detail in Appendix D. The sum $\Delta_c + \Delta_f$ is compared with the value of Δ . The quantity Δ_c is the increase in the cladding inner diameter due to the action of the contact pressure during time period Δt , and the quantity Δ_f is the decrease in the fuel outer diameter due to the same pressure over the same time period. The value of Δ is determined by the following equation

$$\Delta = \Delta D_f - \Delta D_c - G_o , \quad (F4)$$

where

ΔD_f = the increase in fuel diameter during time period due to thermal expansion during a power change or due to fuel swelling during a long period of steady state operation,

ΔD_c = the increase in the cladding inner diameter during time period Δt due to creep, cladding swelling, or both, and

G_o = the size of the fuel-cladding diametral gap at the beginning of time period Δt .

If Δ is negative a fuel-cladding gap still exists. If the sum $\Delta_c + \Delta_f$ is smaller than Δ , the contact pressure is doubled again and the entire process repeated. If the sum is larger, the correct contact pressure has been successfully bracketed, and the bracketed interval is continually divided in half, repeating the calculation each time, until convergence is achieved. Convergence is defined as the point at which the new contact pressure differs from the previous value by no more than 1%.

CREEP calculates the time dependent response of the cladding to the loads imposed upon it. A detailed explanation of the mechanics of this subroutine is contained in Appendix E.

EPLAS calculates the immediate response of the cladding to changes in power level. It is used primarily to determine the thermal strains and stresses, which are then used in CREEP as initial conditions. A detailed explanation of the mechanics of this subroutine is also included in Appendix E.

FEKP calculates the change in fuel geometry due to thermal expansion and fuel swelling. We assume that both thermal expansion and fuel swelling occur isotropically, although a control variable is available to force all swelling and thermal expansion to occur in the radial direction. This control is used for fuel pins employing complete axial restraint. The isotropic assumption is illustrated by the expression

$$\Delta r_1/r_1 = \Delta r_2/r_2 = \Delta h/h = \delta , \quad (F5)$$

where

r_1 = the outer pellet radius,

r_2 = the radius of the central void,

h = the pellet height, and

$\Delta r_1, \Delta r_2, \Delta h$ = changes in pellet radii and height due to swelling and thermal expansion.

Assuming that no volume change distorts the shape of the pellet (i.e., hourglassing or barreling), it can be easily shown, using Eq. (F5), that for isotropic swelling and thermal expansion, two-thirds of the volume change is accommodated by changes in the cross sectional area and one-third of the change accommodated by a change in the pellet height. This relationship is reflected in FEXP.

In FEXP the geometry changes in the fuel pellet are calculated incrementally. At the beginning of a case radial nodes are established for both fuel and cladding (in RADIAL). The initial incremental dimensions are based on cold fuel of as-fabricated fractional density. During irradiation the initial cross sectional area of each radial fuel increment is assumed to be changed by only three factors. The factors are density increase due to fuel restructuring, thermal expansion, and swelling due to fission product accumulation. Restructuring, fuel temperatures, and swelling are calculated elsewhere in the code but are brought together in FEXP to determine the fuel geometry changes. At any point in time during the irradiation history, the cross sectional area of any radial increment will be given by

$$A = A_0(\rho_0/\rho)(1 + 3\alpha T)(1 + X \Delta V/V) , \quad (F6)$$

where

A_0 = the initial cross sectional area, in the as-fabricated condition,

ρ_0 = the initial fractional density,

ρ = the present fractional density,

α = the linear coefficient of thermal expansion,

T = the average temperature of the increment,

$\Delta V/V$ = the amount of fuel swelling due to fission product accumulation,

$X = 2/3$ for isotropic swelling and 1 for complete axial restraint.

Axial extrusion of fuel in the hot plastic region is predicted by FMODEL under some conditions. For example, a pin with a very small fuel-cladding gap that cannot accommodate all the volume change due to swelling and thermal expansion and has not undergone sufficient fuel restructuring to produce a sizable central void, will undergo axial relocation of fuel from the hot central region as radial forces build at the outer surface of this region from mechanical interaction between fuel and cladding. This event is modeled by adjusting the value of A_0 in Eq. (F6) so that the volume change of all radial increments of fuel can be accommodated after the fuel and cladding are in contact.

FMODEL is the main program and is used as a calling program. It also keeps track of the running time for each case and outputs a limited amount of performance information at the end of each case.

FPP calculates the fission gas pressure at the end of a time step. The void volume and volume-average void temperature are calculated, and the fission gas pressure is determined on the basis of the ideal gas law. The number of moles of gas involved is the sum of moles of fill gas plus moles of fission gas. The latter value comes from SWELL. Void volume includes gas plenum, center void, fuel-cladding gap, and fuel porosity.

FUNC1 is part of the gap conductance model. This function calculates the thermal conductivity of a gas mixture, using Brokaw's equation.² See ref. 3 for a complete description of the gap conductance model.

FUNC2 evaluates the integral of the first term of Brokaw's equation with respect to temperature from the cladding inner temperature to the fuel outer temperature. A three-gas mixture is considered; the gases are helium, xenon, and krypton.

FUNC3 evaluates the integral of the second term of Brokaw's equation with respect to temperature from the cladding inner temperature to the fuel outer temperature.

GCON calculates a numerical value for the gap conductance, based upon the cladding inner radius and fuel outer radius input through the argument list. A detailed description of the equations used in this subroutine can be found in ref. 3.

GEE evaluates the temperature jump distances in centimeters at the cladding inner surface and fuel outer surface for the gas mixture contained in the fuel pin. Refer to ref. 3 for additional detail.

GEFCN calculates the fuel temperatures at each radial node using a thermal conductivity expression published by General Electric investigators.⁴ The mechanics of this subroutine are identical to those of a subroutine of the same name in the PROFIL code.⁵

GELB is a subroutine from the ORNL subroutine library. It is used to solve the system of linear equations associated with the cladding stresses and strains (see Appendix E). GELB solves the matrix of equations by Gauss elimination, making use of the highly banded nature of the matrix to improve efficiency.

GSM calculates the volume of fission gas in each radial fuel increment using the Greenwood-Speight model⁶ as modified by Goldberg et al.⁷ GSM is called from SWELL, and the gas volume expressed as $\Delta V/V$ is calculated for one radial increment at a time. Upon return to SWELL the fractional gas release is calculated and applied. Materials constants used in GSM are those used in the FIGRO code.⁷

HUB is the path-controlling subroutine in the FMODEL code. It is essentially a calling subroutine, and very few calculations are performed. Figure F-2 is a simplified flow diagram. HUB is called from FMODEL at the beginning of each cycle in the irradiation lifetime of the fuel pin being studied. The duration of the i th cycle is subdivided into a number of time intervals, and conditions and materials properties are calculated at the beginning of each of these time intervals, and are assumed to remain constant until they are recalculated. The guide to HUB follows:

1. HUB called from FMODEL at beginning of i th cycle;
2. reactor conditions set from input information concerning i th cycle:
 - (a) power factor, (b) coolant temperature, (c) neutron flux, (d) fission rate in fuel, (e) nature of cycle, (f) fission gas pressure (in one-node version);
3. temperature distribution calculated, and mechanical properties of fuel and cladding established, based on the temperature distribution;
4. thermal expansion of fuel and cladding determined, and new gap size calculated;

Fig. F-2. Simplified flow diagram for subroutine RUB.

5. test to see if fuel-cladding gap has closed; if no, go to step 6; if yes, go to step 6a;
6. calculate cladding creep due to fission gas pressure, temperature gradient, and cladding swelling during time increment;
 - a. calculate contact pressure between fuel and cladding,
 - b. calculate fuel and cladding creep due to fuel-cladding contact pressure, temperature gradients, and cladding swelling during time increment;
7. calculate fuel swelling during time increment;
8. calculate fuel restructuring during time increment, recalculating temperature distribution as required (see PVEL);
9. set performance calculations into appropriate arrays for later output;
10. test to see if all time intervals in i th cycle have been considered; if yes, return; if no, go to next time interval (11);
11. go to step 2 and repeat.

INPUT reads data into several arrays contained in COMMON statements. This facilitates a tabulation of all input numbers used in a given case and permits easy addition of input variables without changing the subroutine. An input glossary is included in Appendix B.

KCLAD calculates the temperature distribution in the cladding. Thermal conductivity values for the cladding material are stored in data statements as a function of temperature. These data are from the *Metals Handbook*.⁸ As with the fuel, the temperature calculation at the i th radial cladding node is based upon the temperature at the $i + 1$ node, the thermal conductivity as a function of temperature across the increment, and the heat generation rate within the increment. This method is outlined in the PROFIL code.⁵

LFRAC calculates the stress-rupture life fraction used up during each time interval. Stress-rupture data from pressurized tubes operating under a temperature gradient⁹ are reduced to a Larson-Miller fit, and the life fraction for a time increment is based on the average fission gas pressure or fuel-cladding contact pressure during that time period. This method of estimating cladding damage is probably valid

for the gas plenum region but of limited usefulness in the fueled region of the pin, where fuel-cladding mechanical interaction does not cause damage exactly analogous to damage in pressurized tubes.

MECH determines the fuel and cladding mechanical and physical properties. This subroutine is called immediately after the temperature distribution is calculated, and the properties determined are assumed to remain valid until the next time the temperature distribution is calculated. The fuel elastic and shear moduli and thermal expansion coefficients are calculated from published equations¹⁰⁻¹³ contained in the subroutine. The cladding properties are determined by interpolation from arrays read into the code from INPUT.

PLAST is the basis of the fuel cracking model. Because of the low thermal conductivity of oxide fuels, temperature gradients across the fuel pellet are high, leading to very high thermal stresses. At moderate heat rates the thermal stresses near the pellet surface will exceed the rupture strength of the fuel material, and radial cracks will develop to relieve the stresses. To determine the location of the radial cracks, the stress distribution is calculated across the fuel pellet, assuming that the material is elastic. The technique used for this calculation is the same as is used for the cladding (see EPLAS). The tangential stresses at each radial node are compared with the rupture modulus vs temperature data of Roberts,¹⁴ and the root of the radial crack is assumed to exist at the point where the tangential stress exceeds the rupture modulus. The crack extends from this point to the pellet surface. This method is illustrated in Fig. F-3. The formation of the crack provides two benefits to the calculation. It permits the assumption that the pellet is stress free (the formation of the cracks having relieved the thermal stresses), so that thermal expansion of each radial increment can be determined by the product of the average temperature and the thermal expansion coefficient. In addition, the crack allows a simple evaluation of the response of the fuel to the pressure building at the fuel-cladding interface. It is assumed that the fuel will creep in response to the pressure, and the rate of movement of the fuel surface will be described by the creep characteristics of the fuel at the

Fig. F-3. Rupture modulus vs temperature for UO_2 and $(\text{U,Pu})\text{O}_2$.

roots of the radial cracks. That is, the pressure is transmitted from the fuel-cladding interface to the root of the crack by cracked chunks of cool fuel. This pressure causes the hot plastic core to deform into the central void, or be extruded axially if there is no void.

PLSTR determines the instantaneous response of the cladding to changes in thermal loads that result when the fuel pin linear heat rate changes. PLSTR is called from EPLAS and utilizes the strain-strain technique outlined in Appendix E to estimate the amount of plastic deformation occurring at the cladding node being investigated.

POLY calculates the fuel temperatures at each radial node using a polynomial expansion in temperature to describe the thermal conductivity of theoretically dense fuel. A Maxwell-Eucken or a Loeb correction may be used to correct for existing porosity in the radial increment, with the choice being made by the code user. The calculations made in POLY are identical to those described in the PROFIL code write-up.⁵

PVEL calculates the fuel restructuring that takes place during a given time increment. Nichols' equation¹⁵ for pore migration due to a vaporization-condensation mechanism has been adapted¹⁶ for this purpose. The change in porosity in a given fuel increment is determined by the net movement of pores during the time period in question. Pore velocities are calculated at the inner and outer boundaries of the increment, the pores at the inner boundary moving out of the increment and the pores at the outer boundary moving in. One assumes that the velocities of the pores calculated at the radial nodes are valid throughout the "neighborhood" of the node. This is only approximately correct, however, because the temperatures and temperature gradients calculated at the nodes represent only the nodal points and will vary somewhat in the neighborhood of the node. However, using a small neighborhood keeps the magnitude of this error small. A neighborhood width equal to a third of the increment thickness is built into PVEL. And this convention can be overridden by the code user through the use of input controls, with the user providing his own value for the size of the neighborhood.

Grain growth is also calculated in SUBROUTINE PVEL. We feel the influence of grain size of fuel material on fission gas release, swelling, and Nabarro-Herring creep of mixed oxide fuels will be quite important, and we have therefore included sophisticated procedures for calculating changes in grain size during irradiation in FMODEL. To develop the equations to describe in-reactor grain growth of $(U,Pu)O_2$, data for two low-burnup pins were combined and analyzed as shown in Fig. F-4. The least-squares equations given in the figure relate to the observed grain size in micrometers (D), to the initial grain size (D_0), the irradiation time in hours (t), and the irradiation temperature in degrees centigrade (T). In the higher temperature region, solid fission products or gas bubbles retard the rate of grain growth. The in-reactor activation energies are smaller than expected from out-of-reactor grain growth of UO_2 and ThO_2 . To determine if the lower temperature dependence was typical of the mixed oxide or was an irradiation effect, out-of-reactor grain growth rates of $(U,Pu)O_2$ were determined. The out-of-reactor data are also of value in estimating the thermal treatment necessary to fabricate fuel of a specified grain size should it be required.

Fig. F-4. Grain growth of $U_{0.85}Pu_{0.15}O_2$ in-reactor.

The out-of-reactor grain growth study was conducted with sol-gel $U_{0.85}Pu_{0.15}O_{2.00}$ microspheres made by the same process used to make the fuel examined in the in-reactor study but from a different batch. The samples were heated isothermally in Ar-4% H_2 at 1200, 1356, and 1550°C for times up to 164 hr. The grain size is plotted as a function of annealing time in Fig. F-5. Also shown in Fig. F-5 for comparison are curves for 1356 and 1550°C calculated from the in-reactor grain growth results. At 1356°C the in- and out-of-reactor results are similar; at this temperature irradiation may have increased the rate of grain growth. At 1550°C comparison of the in- and out-of-reactor results shows conclusively that grain growth was retarded by irradiation, perhaps as a result of the presence of fission gas bubbles or solid fission product inclusions.

Fig. F-5. Grain size as a function of time for $U_{0.85}Pu_{0.15}O_2$ isothermally annealed out-of-reactor at 1200, 1356, and 1550°C.

Least-squares analysis of the out-of-reactor data yielded the equation

$$D^2 - D_0^2 = 2.52 \times 10^{21} t \exp(-173,000/RT).$$

The value for the activation energy (173 + 25 kcal/mole at the 90% confidence level) is comparable to values observed out-of-reactor for UO_2 and ThO_2 , but is considerably larger than the values of 29.2 and 5.96 observed in-reactor. This demonstrates that data obtained from isothermal out-of-reactor tests cannot be used to predict in-reactor grain growth $(U,Pu)O_2$.

Component redistribution is also computed within SUBROUTINE PVEL. The actinide redistribution models are intimately linked to the fuel restructuring model. The vaporization-condensation model for pore

migration envisions fuel material being vaporized from the hot side of the pore and condensing on the cold side, resulting in net movement of the pore up the temperature gradient. However, in a mixed-oxide fuel containing both uranium and plutonium, the composition of the vapor is not necessarily the same as that of the solid material present at the hot side of a pore. It may be rich in uranium or rich in plutonium, depending on the local oxygen-to-metal ratio. So there is a net movement of uranium or plutonium away from the central void region. To compute the amount of actinide redistribution during any given period of time, it is necessary to first predict changes from the initial oxygen-to-metal ratio. This is done through an irreversible thermodynamic approach, which has been previously described.¹⁷ The details of this calculation and of the actinide redistribution are contained in a recent paper¹⁸ and will not be repeated here.

RADIAL calculates the size of the fuel and cladding increments at the beginning of each case. The cold dimensions of the fuel and cladding are used in the calculation. The user has the choice of using increments of equal thickness or equal volume or reading in the radial locations of each node. An input control variable is used to make this choice.

RELAX calculates the fuel-cladding mechanical interaction when a power change takes place "instantaneously" so that there is not time for fuel or cladding creep to relax the interaction. The calculation is accomplished by determining the differential thermal expansion that would occur if there was no interaction and then forcing the cladding to instantaneously accommodate the difference through plastic deformation as well.

RELEASE calculates the fraction of fission gas released as a function of temperature alone. It is assumed that the fission gas is released when formed; therefore this is a steady-state event rather than a burst of gas released during a shutdown or power reduction. Temperature-release pairs are input to control the gas release calculation.

RPP established the radial power profile for thermal flux irradiations. Provision is made for changing the radial power profile with burnup. The current version of this subroutine reflects the anticipated changes in the radial power profile with burnup for the MINT-2 test,¹⁹ and data for the relative power as a function of radial position and burnup are stored in data statements. To use FMODEL to analyze a thermal flux irradiation with characteristics different from MINT-2 would require some modifications to this subroutine.

SET1 sets the correct values of stress and strain into the appropriate common area arrays before entry into CREEP. This is necessary because of the iterative nature of the fuel-cladding mechanical interaction analysis. CREEP is called during each iteration, and the stress-strain arrays are filled with numbers that may or may not be useful later in the calculation. When convergence is attained, the stress-strain values associated with the "correct" solution are stored for later use.

SET2 sets the correct values of elastic modulus, Poisson's ratio, and temperature into the appropriate arrays before entry into EPLAS and CREEP. This is necessary because fuel and cladding temperatures may be changing constantly, requiring a recalculation of these temperature-dependent properties. In addition, EPLAS and CREEP employ a system of nodal points that is different to that employed elsewhere in the program.

SET4 sets values from the input arrays into other common area arrays.

STDFCN calculates fuel temperatures at each radial node using a standard-form thermal conductivity function with empirical constants taken from Sayles²⁰ and a porosity correction term suggested by Biancheria.²¹ The mechanics of this subroutine is identical to that of a subroutine of the same name in the PROFIL code.⁵

STR calculates the creep rate of the fuel in response to the stress condition resulting from fuel-cladding mechanical contact. Two forms of the creep equation are available, both based on data taken from testing of UO₂ out-of-reactor. We generally use the Bohaboy²² equation for high-density fuel, but since it is not valid below densities of about 92% of theoretical, for more porous fuels we use the equation

suggested by Clauer.²³ Since the creep rate of mixed oxide fuel depends upon the grain size, Lackey's grain growth equation (see PVEL) is used to determine the change in grain size with time.

SWELL calculates fuel swelling due to fission product accumulation. Both solid and gaseous fission products are considered. A constant swelling rate due to solid fission products is used, and the volume of fission gas bubbles is calculated in GSM. A fraction of the fission gas bubble volume is assumed to be released upon formation of the bubbles and therefore does not contribute to fuel swelling. A fraction of the fabricated porosity is assumed available to accommodate fission products, as previously described.²⁴ Since the magnitude of the fuel-cladding contact pressure will influence the volume of fission gas bubbles, SWELL is included in the iteration to determine the contact pressure. There will be little influence of fuel swelling on the fuel-cladding contact pressure due to differential thermal expansion during startup, but the contact pressure due to fuel swelling during steady-state operation will be strongly influenced.

TAVG calculates the average temperature in a fuel increment, based on the temperatures at the outer and inner boundaries of the increment.

TDIST calculates the temperature distribution across the axial segment being considered. The calculation begins with the coolant temperature and proceeds to the cladding outside by calculating the temperature rise across the cladding film. Using cladding thermal conductivity values obtained from KCLAD, the temperature rise across the cladding is calculated. Then using a gap conductance value obtained from GCON (or input by the user if so desired) the temperature rise across the fuel-cladding gap is calculated. Once the fuel surface temperature is known, the temperature distribution across the fuel pellet is done as in PROFIL⁵ except that the fuel restructuring model described in Appendix C is used rather than the three-ring version used in PROFIL. After the fuel temperature distribution has been calculated, thermal expansion of the pellet is calculated in FEXP so that the gap size can be recalculated. This iterative process is repeated until the present and previously calculated fuel surface temperatures agree to within 1°C.

XINTB linearly interpolates between values in arrays.

XPLSTR computes the increment of creep strain that occurs during a creep time interval. It is called from CREEP, and the details of the calculation are presented in Appendix E.

YPICK picks a value of Y corresponding to an input value of X for a function of the form $Y = mX + b$ where m is the slope and b the Y -axis intercept of the equation.

ZERO places a zero in every common area storage array at the beginning of each case. Only dimensioned common locations are filled with zeros.

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