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FISSION GAS RELEASE (FGASRL)

RICHARD E. MASON

March 1978

EG&G Idaho, Inc.

IDAHO NATIONAL ENGINEERING LABORATORY

DEPARTMENT OF ENERGY

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Idaho National Engineering Laboratory
Idaho Falls, Idaho 83401
operated by
EG&G Idaho, Inc.
for the
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PRELIMINARY ANALYSIS REPORT

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FISSION GAS RELEASE (FGASRL)

R. E. Mason

REVIEWED BY:

D. L. Hagrman

D. L. Hagrman
Section Leader

Michael P Bohn

M. P. Bohn, Manager
FARAD Branch

APPROVED BY:

Paul North

Paul North, Manager
Code Development and
Analysis Program

EG&G IDAHO, INC.

FOREWORD

This report describes work which is part of the fuel rod behavior modeling carried out at EG&G Idaho, Inc. It is an interim addition to work previously published in MATPRO Version 09 - A Handbook of Materials Properties for use in the Analysis of Light Water Reactor Fuel Rod Behavior, TREE-NUREG-1005 (December 1976), and will replace Section 12, Appendix A.

The material property correlations and computer subcodes described in MATPRO are developed for use in light water reactor (LWR) analytical programs such as the Fuel Rod Analysis Program -- Steady-State (FRAP-S3) code. This work is performed as part of a broad effort to develop and verify analytical models capable of describing nuclear fuel rod behavior.

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12. FISSION GAS RELEASE (FGASRL)

(R. E. MASON)

During irradiation of water reactor fuel rods, gaseous fission products are produced in the fuel and are slowly released to various void volumes in the fuel rods. The released fission gases degrade the initial fill gas thermal conductivity and thus change the thermal response of the fuel rods. Moreover, fuel rod internal pressure is increased so that the cladding mechanical response is affected.

The fission gas release subcode FGASRL is intended for use in analytical codes which predict water reactor fuel pin behavior. The development effort was directed primarily at improving code predictions of the gas release model used in FRAP-S3 which overpredicts^[A-12.1] release of fuels irradiated at relatively low operating temperatures and therefore small gas release fractions.

12.1 Summary

The fission gas release subcode (FGASRL) presented in this report describes a two-step gas release process: (a) Fission gas release from fuel grains to the grain boundaries and, (b) fission gas release from the grain boundaries to internal free volume of the fuel pin. The fission gas reaching the fuel pin free volume is a fraction (F) times the sum of the fission gas stored at the grain boundaries (S) and the fission gas that reaches the grain boundaries (Δn) during a time increment

$$R = F (S + \Delta n) \quad (A-12.1)$$

where

R = fission gas released to the fuel pin free volume (mol)

F = fraction of fission gas released from the grain boundaries to the fuel pin free volume

S = fission gas stored at the grain boundaries during previous time steps (mol)

Δn = fission gas released from fuel grains to the grain boundaries during a time increment (mol).

The fraction of grain boundary gas released to the pin free volume is a function of fuel density and grain size and is calculated in FGASRL using the equations

1) for $T \leq 2100$ K

$$F = 1 - \text{erf}(\rho) + \exp(-1.25 \times 10^{14}/B^3) \quad (\text{A-12.2a})$$

2) for $T > 2100$ K

$$F = 1 - [\text{erf}(\rho)/(T - 2100)] + [\exp(-1.25 \times 10^{14}/B^3)] \quad (\text{A-12.2b})$$

where

F = the fraction of fission gas released from the grain boundaries to the fuel pin free volume.

$$\rho = 1.0/[1.0 + 10^5 (1.0/X - 1.0)/g^3]$$

X = fractional fuel porosity

B = burnup (MWd/t)

g = average grain diameter (μ)

T = fuel temperature (K)

erf(ρ) = error function

where

$$\text{erf}(\rho) = \frac{2}{\sqrt{\pi}} \int_0^\rho e^{-t^2} dt.$$

The fission gas reaching the grain boundaries from the fuel grains is calculated using the equation

$$\Delta n = \beta \left[t - \frac{[1 - \exp(k' k'' t)] (1 - k')}{k' k''} \right] + C [1 - \exp(k' k'' t)] \quad (\text{A-12.3})$$

where

Δn = fission gas released from the grain matrix to the grain boundaries (mol)

β = fission gas production rate (mol/s)

t = time step (s)

C = fission gas trapped at defect sites in the grain matrix at the beginning of the step (mol)

$$k' = 9 \times 10^7 \exp(-45\,289.9/T) + 0.0005$$

T = fuel temperature (K)

$$k'' = 0.0005 \left\{ 1 - 1/\left[\exp\left(\frac{T - 1900}{40}\right) + 1\right] + \exp\left(1.24 \times 10^{14}/B^3\right) \right\}$$

B = total burnup (MWd/t).

Equations (A-12.1), (A-12.2), and (A-12.3) describe the subcode calculation of fission gas release from water reactor fuel. The resulting correlation is a function of temperature, time, burnup, grain size, and fuel density. Time steps of 7.9×10^6 s (2200 hr) or less are to be used when making FGASRL gas release calculations. FGASRL fractional gas release prediction (the fraction of total fission gas released to total produced) using a fuel rod operation history is within $\pm 60\%$ of the fractional gas released experienced by the fuel rod.

Section 12.2 of this report describes the development of the subcode. In Section 12.3 a comparison of subcode predictions with gas release data is discussed along with predictions of the GRASS code. Section 12.4 provides the computer programming listings of the FGASRL subcode and Section 12.5 contains the references.

12.2 Model Development

Fission gas release from nuclear fuels results from a number of physical processes. The author assumed that gas release is controlled in two major steps, shown schematically in Figure A-12.1. These processes are further assumed to occur in series. The fission gas created in a grain either migrates to the grain boundary or is trapped in the grain interior by grain defect traps until it is released and migrates to the grain boundaries. Fission gas reaching the grain boundaries is stored there or released to the fuel pin free volume.

12.2.1 Analytical Model Development. Following Weisman et al.^[A-12.2], the various mechanisms for gas release from the grains to the grain boundaries [i.e., recoil and/or knockout by fission fragments passing through the grains^[A-12.3], random motion^[A-12.4], biased movement^[A-12.5] (due to temperature gradient), etc.] are represented simply as a single type of gas movement through the grain. This representation corresponds with the escape of the gas from the fuel grains to the grain boundaries. Two probabilities in evaluating fission gas release from grains are defined. The first, k' , is the probability of direct release from the

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Fig. A-12.1 Schematic of the mechanisms modeled in the FGASRL fission gas release model. The shaded areas represent fuel grains and the open areas represent pores or gas bubbles. The fission gas is created in a grain (a) and then migrates to the grain boundaries (c) or migrates (b) to grain defect traps (d). Trapped atoms are eventually released back into the grain matrix (e) and diffuse to the grain boundaries (f). Fission gas is trapped at the grain boundaries until it is released (g) through fissures or cracks (h) communicating with the fuel pin free volume.

fuel grains to the grain boundaries, and the second, k'' , is the probability of release per unit time of fission gases from grain defect traps such as dislocations, large bubbles, etc [A-12.5, A-12.6].

If β is the gas production rate, then the rate of direct gas release to the grain boundaries of gas created during a time step, t , is $\beta k'$. If C is the number of gas moles that are trapped in the grain matrix, the rate of release from the trap is $C k''$. The gas released from the traps escapes from the interior of the grain to the grain boundary by the same process as the newly created gas. The total rate of fission gas release from the interior of the grain to the grain surface is

$$\frac{dn}{dt} = k' (\beta + k''C) \quad (A-12.4)$$

where

n = fission gas released from the grain interior to the grain surfaces (mol)

β = fission gas production rate (mol/s)

C = fission gases in the trap (mol)

t = time (s)

k' = probability of direct release from the grains

k'' = probability per unit time of release of fission gases from grain defect traps.

The rate of fission gas production in the fuel matrix during steady state is equal to the sum of the rate of loss from the matrix to the grain surfaces and the loss to the interior grain defect traps or

$$\beta = \frac{dn}{dt} + \frac{dC}{dt} \quad (A-12.5)$$

For any period of time in which β , k' , and k'' are approximately constant, Equations (A-12.3) and (A-12.4) may be solved simultaneously^[a] to show:

$$\eta_i - \eta_{i-1} = \beta_i \left[t_i - \frac{(1 - k'_i)}{k'_i k''_i} [1 - \exp(-k'_i k''_i t_i)] \right] + C_{i-1} [1 - \exp(-k'_i k''_i t_i)] \quad (\text{A-12.6})$$

where

η_i = fission gas released from the grain during the time step interval, t_i .

η_{i-1} = fission gas released from the grain at $t_i = 0$

t_i = length of the time interval

k'_i and k''_i = values of k' and k'' during the time interval

C_{i-1} = fission gas in the trap at the start of the time interval.

k' was assumed to have an Arrhenius temperature dependence. This functional form is reasonable because the probability of escape by diffusion without being trapped is quite small at low temperatures but rises rapidly at high temperatures^[A-12.3, A-12.7, A-12.8]. An additional constant term (H) was included in the expression for k' to represent the temperature-independent contribution of knock-out and recoil.

$$k' = A \exp(-Q/T) + H \quad (\text{A-12.7})$$

[a] $\frac{dn}{dt}$ is eliminated and the integrating factor $e^{k' k'' t}$ is used to find C . A similar integration of Equation (12.4) with the solution for C substituted yields Equation (A-12.6).

where

T = temperature (K)

A, Q, H = constants.

The constants A , Q , and H were determined by fitting the model to gas release data as explained later in this section.

The probability function k'' simulates fission gas release observed across the radius of a fuel pellet^[A-12.9]. The equation used to represent the observed radial gas release distribution is

$$k'' = g(1.0 - 1.0 / \left[\exp\left(\frac{t - h}{\ell}\right) + 1 \right] + \exp\left(\frac{1.25 \times 10^{14}}{B^3}\right)) \quad (A-12.8)$$

where

k'' = probability that gas will be released from grain trapping sites

T = fuel temperature (K)

g, h, ℓ = constants

B = burnup (MWd/t).

The term containing the burnup was included to model enhanced fission gas release observed at high burnups ($> 35,000$ MWd/t)^[A-12.10] and is an empirical fit to enhance the fission gas release burnups above 30,000 MWd/t.

After the fission gas reaches the grain boundaries, it can be released through pores (interconnected tunnels) that are open to the pin free volume. While fission gas diffusion and migration of grain boundaries may assist in the accumulation of fission gases, the movement of fission gases from grain boundaries is associated more with mechanical changes

in the fuel [A-12.11, A-12.12]. As pointed out by Olander [A-12.13], grain boundary fission gas release occurs in one of two ways: (a) by bubble interlinkage to the cracks or other fissures communicating with the fuel pin free volume or, (b) communication of the gas bubbles with the free volume because of stress cracking of the fuel pellet. A model for gas storage and release from grain boundaries was developed using a simplified version of the pore percolation theory [A-12.14] and a statistical distribution function similar to that used in the GRASS code [A-12.15]. This method considers only the first of the two grain boundary release mechanisms described above. The statistical distribution function used in the FGASRL subcode is

$$F = \frac{\sqrt{2}}{\sqrt{\pi} \sigma} \int_{\rho}^{\infty} \exp\left(-(x - \rho)^2 / 2\sigma^2\right) dx \quad (A-12.9)$$

where

F = fractional fission gas release from grain boundaries

σ = constant

ρ = microstructure parameter

The parameter ρ is a function of porosity such that as the porosity increases, ρ increases and as the grain size increases, the gas stored in the grain boundaries increases. The resulting microstructure parameter is

$$\rho = 1 / \left\{ 1 + a \left(\frac{1}{X} - 1 \right) / g^3 \right\} \quad (A-12.10)$$

where

ρ = probability parameter

a = constant (μ^3)

g = grain diameter (μ).

X = fractional porosity.

Evaluating Equation (A-12.9) between the limits shown gives

$$F = 1 - \text{erf}(\rho) \quad (\text{A-12.11})$$

Here as with the k'' function of Equation (A-12.7), a high burnup term was added to Equation (A-12.12) to predict the enhanced gas release observed in the high burnup fuel discussed by Baroch and Rigdon^[A-12.10]. The function is

1) for temperatures ≤ 2100 K

$$F = 1 - \text{erf}(\rho) + \exp(-1.25 \times 10^{14}/B^3) \quad (\text{A-12.12})$$

2) for temperatures > 2100 K

$$F = 1 - \text{erf}(\rho)/(T - 2100) + \exp(-1.25 \times 10^{14}/B^3) \quad (\text{A-12.13})$$

where

T = fuel temperature (K)

ρ = parameter defined in Equation (A-12.10)

B = burnup (Mwd/t).

The equation above corresponds in principle with Turnbull's^[A-12.16] conclusion that release of krypton increases as the grain size of the fuel increases.

The model for stored grain boundary fission gas release is especially relevant to reactor transient condition as has been demonstrated by the transient heating tests conducted at Argonne National Laboratory^[A-12.17]. There it was found that under reactor transient conditions the fuel cracking

takes place along the grain boundaries, releasing both the gas trapped at the grain boundaries and the gas that was able to diffuse to the grain boundaries during the transient. A similar effect was observed in the transient tests at the Idaho National Engineering Laboratories in the film boiling regime^[A-12.18]. To provide this "grain boundary stored gas" to transient calculations, the equations described above were included in the FGASRL gas release calculations.

12.2.2 Evaluation of Constants. In order to evaluate the constants in Equations (A-12.1) and (A-12.2), the subcode was correlated with non-proprietary fission gas release data of water-moderated reactor. The data selection criteria were that the approximate centerline temperature of the irradiated fuel be documented, that the operational history be documented in enough detail to be used in the FRAP-S3^[A-12.19] analytical code, and that the fission gas release be documented. These criteria were used by the author because the subcode is to be used to predict the gas release from such fuel rods and must be able to do that with the fuel pin histories available. Using the criteria above, four fuel assemblies were chosen and, from those four assemblies, five rods were chosen to use in evaluating the constants in the equations.

The AECL 2230^[A-12.20] fuel rod and the AECL 1676^[A-12.21] fuel rod data are especially useful in determining the equation constants because they were irradiated at a relatively constant power ($\leq 20\%$ power variation)^[A-12.22]. The rest were chosen because of their temperature or burnup range. Barach and Rigdon^[A-12.10] have reported fission gas release data for Babcock & Wilcox (B&W) fuel irradiated up to 80,000 MWd/t, but a complete irradiation history is not documented. Because the Baroch and Rigdon data is the only nonproprietary data of thermal reactor fuel irradiated to high burnups with corresponding enhanced gas release, their data were used to correlate the subcode for high burnups.

The fission gas release data used in evaluating the constants of the FGASRL subcode are listed in Table A-12.I. The table includes the literature source of the data used, the fuel burnup reached, and the average power of the fuel. Also listed are the FRAP^[A-12.19] calculated

TABLE A-12.1

DATA USED TO EVALUATE CONSTANTS IN FGASRL

Reference	Source	Rod	Burnup (MWd/t)	Average Density (kg/m ³)	Peak Power (kW/ft)	Grain Size (μ)	Fuel Centerline Temperature		Fission Gas Release
							FRAP	Experimental	
A-12.23	SAXTON II	B	15896	10.3×10^3	46.3	5.0	2847	2473	36.0
A-12.20	AECL 2230	CBX	2710	10.4×10^3	8.1	5.0	2380	2293	18.8
A-12.21	AECL 1676	DFA	344	10.7×10^3	57.1	5.0	2560	2001	4.6
A-12.10	B&W ^[a]	7	56581	10.3×10^3	52.5	5.0	2450	2216	71.9
A-12.10	B&W ^[a]	33	35500	10.3×10^3	62.3	5.0	2871	2060	27.4

[a] Babcox & Wilcox data reported by Baroch and Rigdon^[A-12.10]

centerline temperature and the centerline temperature reported in the literature, the fractional gas release and the initial fuel grain size. The fission gas release data listed in Table A-12.1 are by no means all the gas release data that are available. Additional data which may be useful for further model development are listed in References A-12.25 to A-12.42.

Derivation of the constants in the expression for k' [Equation (A-12.7)] was based on the assumption that movement of fission gas atoms from the fuel grains to the grain boundaries is diffusion controlled. The probability that the gas atoms will reach the grain boundaries k' without being trapped was assumed to be an Arrhenius function.

The constant Q of Equation (A-12.7) was taken to be a number similar to the diffusional activation energy of fission gases in water reactor fuels. Activation energies for gas movement, bubble movement, etc. reported in the literature range from $\sim 83\,720$ J/mol to $\sim 5.65 \times 10^5$ J/mol [A-12.42, A-12.7, A-12.13]. For the calculations described in this report, Q was chosen to be 3.767×10^5 . Using this value and adjusting the other constants of Equation (A-12.6) to fit the experimental fuel rod gas release data, the final k' function is

$$k' = 9 \times 10^7 \exp(-45\,289.9/T) + 0.0005 \quad (\text{A-12.14})$$

where

T = fuel temperature (K).

The probability per unit time that fission gas will be released from the defect trapping sites in the grains, k'' , was assumed to be a Fermi function^[a]. The constants of Equation (A-12.8) were chosen so that

[a] The Fermi function is defined as

$$f(t) = 1 / \left[\exp\left(\frac{T - T_0}{\Delta T}\right) + 1 \right]$$

where T_0 and ΔT are constants and T is the fuel temperature.

fission gas release will increase rapidly in the temperature range of 1600 to 2000 K. This temperature range corresponds to the reported fuel temperature in regions of fuel pellets examined by Argonne National Laboratory which showed a sharp decrease in fuel fission gas retention^[A-12.9]. The final form of the k'' term is

$$k'' = 0.0001 \left\{ 1.0 - 1.0 / \left[\exp\left(\frac{T - 1900}{40}\right) + 1 \right] + \exp\left(\frac{-1.25 \times 10^{14}}{B^3}\right) \right\}. \quad (A-12.15)$$

k'' is then the term of Equation (A-12.3) that causes the prediction of low gas release from the fuel grains at low temperatures and rapidly increasing release between fuel temperatures of 1800 K and 2500 K depending on the magnitude of the time step. The burnup term on the right side of Equation (A-12.15) is a purely empirical function added to model the enhanced gas release seen at large burnups (>35 000 Mwd/t). It affects the calculations only above 30 000 Mwd/t.

The remainder of this section is a discussion of the behavior of Equation (A-12.5) using the constants discussed. The first term on the right side of Equation (A-12.5) is

$$\beta_i \left[t_i - \frac{(1 - k_i') [1 - \exp(-k_i' k_i'' t_i)]}{k_i' k_i''} \right]$$

which represents the number of gas atoms created during the time step, t_i , that escape to the grain boundary and are not trapped within the fuel grain. This can be reduced to a ratio of those gas atoms created and subsequently released to the total fission gas atoms created in time step t_i . This fractional release ratio is

$$F_B = 1 - \frac{(1 - k_i') [1 - \exp(k_i' k_i'' t_i)]}{T_i k_i' k_i''}. \quad (A-12.16)$$

The fraction, F_B , is plotted as a function of temperature in Figure A-12.2 for various times. Figure A-12.2 shows that for temperatures below 1600 K the gas release fraction is less than 0.001 and approaches total

Fig. A-12.2 Temperature dependence of the terms in Equation (A-12.1).

gas release at temperatures above 2200 K for long time steps. For time steps less than 200 hr, it approaches total gas release at ~ 2500 K. The second term on the right side of Equation (A-12.3), $C [1 - \exp(k'k''t)]$, is in effect the number of trapped gas moles that escape to the grain boundary during a time step t . This can be expressed as a fractional release of the number of moles trapped in the fuel grains.

$$F_C = 1 - \exp(k'k''t). \quad (A-12.17)$$

The fraction F_C (dashed lines) is also plotted in Figure A-12.2. Fission gas release from traps is similar to the release from the matrix (F_B). However at temperatures in the range of 1700 to 2100 K, the trap release fraction is larger than the matrix release fraction.

The technique used to find constants in the expression for the calculation of the parameter ρ [Equation (A-12.10)] was simply to choose constants for the equation such that, (a) ρ ranged from 0 to 1 for grain sizes between 1 and 500 microns, and (b) the fractional grain boundary release depicted in Figure A-12.3 was produced.

The constant, a , of Equation (A-12.10) is 10^5 and the resulting equation to determine ρ is

$$\rho = 1 / \left\{ 1 + 10^5 \left(\frac{1}{X} - 1 \right) / g^3 \right\} \quad (A-12.18)$$

There were no direct numerical data to correlate these results with, but (as discussed previously) the effect is important enough for it to be included in the subcode calculations.

12.3 Comparison with Data and GRASS Code Predictions

The calculated values of the subcode developed in Section 12.2 are discussed in this section and are compared to the appropriate experimental data. The FGASRL subcode and experimental data are also discussed relative to the predictions obtained with the GRASS code [A-12.14].

Fig. A-12.3 Fractional gas release from the grain boundaries to the fuel pin free volume.

Figure A-12.4 shows the correspondence of the FGASRL subcode to its data base and to data not used to develop the model. Because of the complexity of fission gas release mechanisms and the nonlinear functions used in the FGASRL subcode, the uncertainty of the code predictions is as the standard error of the percent difference of the FGASRL fractional fission gas release prediction divided by the experimentally determined fractional fission gas release. That is

$$SE = \sqrt{\sum_{i=1}^N \left(\frac{P_i - E_i}{E_i} \right)^2} \frac{1}{N} \quad (A-12.19)$$

where

SE = standard error of prediction

P_i = FGASRL fractional gas release prediction (%)

E_i = experimentally determined fractional gas release (%)

N = number of data used.

Using the formulation above, the uncertainty of the FGASRL predictions was found to be accurate to within $\pm 60\%$ of the experimentally determined values. The dashed lines shown in Figure A-12.4 depict the uncertainty bands of the FGASRL predictions. The new gas release model is a significant improvement over the previous gas release model which had a standard error of $\pm 420\%$ using the same data base and uncertainty determination method. At higher fractional releases, considerable uncertainty exists but this prediction accuracy is probably as good as can be expected even with more sophisticated gas release codes using the present state-of-the-art gas release prediction methods and the present knowledge of fission gas release processes.

An important new feature of the revised FGASRL model is the inclusion of grain boundary storage. Sample calculations of grain boundary stored fission gas determined during a FRAP-FGASRL calculation of gas

Fig. A-12.4 FGASRL fission gas release predictions compared to the release reported in related studies.

release are shown in Figure A-12.5. The lines in the figure represent the stored gas (in moles) in two specific fuel sections. The dashed line represents the gas stored in a ring which is at the center of the fuel column near the top of the fuel rod. Fission gas stored at this location gradually increases with increasing irradiation time and increasing grain size up to about 5000 hours. The solid line represents fission gas stored at a fuel ring halfway between the center of the fuel and the fuel edge and shows a relatively constant quantity of fission gas at the grain boundaries. The fraction of gas stored at each location shown in Figure A-12.5 is primarily a function of the gas produced during a time step and the amount that reaches the boundaries from the grain. That is, at higher irradiation powers more gas is released from the grain and grain boundary storage increases, but as power decreases this stored gas decreases as gas is being removed faster than it is being replaced.

The effect of the burnup term of Equation (A-12.2) and Equation (A-12.7) on the gas release predicted by the FGASRL subcode is shown in Figure A-12.6. The subcode calculations were made assuming isothermal fuel temperatures of 1500 K (solid line) and 1800 K (dashed line) and using time steps of 7.2×10^6 s and 75 micron fuel grains. The solid line shows the minimum gas release calculated by the subcode at burnups above 30 000 Mwd/t. The dashed line shows the added gas release calculated for fuel at temperatures above ~ 1500 K. FGASRL predictions for high burnups produces releases of the same magnitude as the data reported and each experimental value reported can be directly correlated with FGASRL predictions using an accurate power and temperature history.

The GRASS subroutine^[A-12.14] has been examined and a driver developed to run the subcode on the CDC computer at Idaho National Engineering Laboratory (INEL). The driver provides the GRASS code with a "cosine function" power and temperature distribution and the other parameters required to run the GRASS code. The time steps are calculated in the driver program to begin in very small increments (~ 10 hr) increasing on a percent of total run time specified until the desired irradiation time is reached. Using this code driver, a preliminary comparison of the GRASS code and the FGASRL code was completed.

Fig. A-12.5 An example of the fission gas stored at the grain boundaries as calculated by the FGASRL subcode. Each line represents the number of moles stored in a section of the fuel.

Fig. A-12.6 FGASRL gas release predictions compared to Babcock & Wilcox (B&W) gas release data.

The AECL-2230 (CBX) rod operational parameters and a total irradiation time of 7.01×10^6 s (1948 hr) were used to compare the GRASS code to experimental data. A total fractional release of ~2% was calculated with the GRASS code. This is significantly lower than the 18.8% reported for the CBX rod. The irradiation history was not followed exactly in this calculation but since this rod was operated at a relatively constant power, it does represent a good approximation. Figure A-12.7 shows the fractional gas release as a function of power and temperature. This can be compared with FGASRL predictions from Figure A-12.2 which are repeated in Figure A-12.7.

The fractional release calculation at 72 kW/m of power demonstrates the differences between FGASRL and GRASS. The gas release function calculation of FGASRL and GRASS begin increasing around 1800 K but the FGASRL fractional release curve is much steeper and reaches unity much earlier than the GRASS fractional release does. The two lower power curves show very little release increase over the temperature range considered.

12.4 FORTRAN Subcode

A listing of the computer subcode FGASRL is presented in Table A-12.II and the FGASRL update used in the FRAP-S3 analytical code is presented in Table A-12.III.

Fig. A-12.7 Fractional fission gas release predictions calculated by the GRASS subcode. The time step was 1.36×10^6 s (379 hr).

TABLE A-12.II

LISTING OF THE FGASRL SUBCODE

PROGRAM RIKCHK(INPUT, OUTPUT, TAPE 6 = OUTPUT)
SUBROUTINE FGASRL (FTEMP, TIME, BU, FDENS, GRNSIZ, FMGPR, L, IT,
CC2, GBBG, FMGR)

FGASRL CALCULATES THE FISSION GAS RELEASE AS A FUNCTION
OF TEMPERATURE, FUEL POROSITY, TIME, GRAIN SIZE, AND BURNUP.

- INPUT -

FTEMP = FUEL RING AVERAGE TEMPERATURE (DEG K)
FDENS = FUEL DENSITY (KILOGRAMS/CUBIC METER)
TIME = TIME AT TEMPERATURE (SEC)
BU = FUEL BURNUP (MEGA-WATT-SEC/KILOGRAM METAL OXIDE)
GRNSIZ = FUEL GRAIN SIZE (MICRONS)
FMGPR = FISSION GAS PRODUCED IN THE J FUEL RING (MOLES)
L = FUEL RING INDEX (1 - 10)
IT = POWER STEP

- OUTPUT -

CC2 = CONCENTRATION OF GRAIN TRAPPED FISSION GAS
PER RING (MOLES)
GBBG = CONCENTRATION OF GRAIN BOUNDARY TRAPPED FISSION
GAS PER RING (MOLES)
FMGR = CUMULATIVE FISSION GAS RELEASE PER INCRUMENT

FGASRL = WAS CODED BY R. E. MASON IN MARCH 1978

THE FGASRL CORRELATION WAS BASED ON THE FOLLOWING DATA

M.J.F.NOTLEY AND J.R.MACEWAN, ORNL AECL - 2230
M.J.F.NOTLEY, ET AL., AECL - 1676
W.R.SMALLEY, WACAP - 3385 - 56
C.E.BEYER AND C.R.HANN BNWL - 1876

TABLE A-12.II (continued)

```

C      DIMENSION GBBG(11), FMGR(11), CC2(11), FMGPR(11), GRNSIZ(11)
C
C      AN APPROXIMATION FOR THE ERROR FUNCTION WAS USED TO EVALUATE
C      THE CONSTANTS IN THE FOLLOWING EQUATIONS
C      THE APPROXIMATION WAS TAKEN FROM
C      C.H.HASTINGS,JR., APPROXIMATIONS FOR DIGITAL COMPUTERS
C      PRINCETON UNIVERSITY PRESS 1955
C
C      ERF(X) = 1.0 - 0.348024 * 1.0/(1.0 + 0.47047 * X) +
=      0.0958798 * (1.0/(1.0 + 0.47047 * X)) **2.0 -
=      0.7478556 * (1.0/(1.0 + 0.47047 * X)) ** 3.0 + 0.000025
C
C
C      - PROGRAM -
C
C      INITIALIZATION
C
C      IF(IT .EQ. 1) GBBG(L) = 0.0
C      IF(IT .EQ. 1) FMAA    = 0.0
C      IF(IT .EQ. 1) FMGR(L) = 0.0
C      IF (IT .EQ. 1) CC2(L) = 0.0
C      IF(BU .LE. 0.0) BU = 1.0
C
C      CALCULATION OF THE HIGH BURNUP FACTOR
C
C      BUNKEL = 1.25E14/((BU / 86.4) ** 3.0)
C      IF(BUNKEL .GE. 400.0) BUNKEL = 400.0
C
C      CALCULATION OF FUEL GRAIN RELEASE
C
C      AK1      = 9.0E 07 * (EXP(-45289.86/FTEMP)) + 0.0005
C      AK2      = 0.00005 * AK1 * (1.0 - 1.0/(EXP((FTEMP - 1900.0)/40.0)
=      + 1.0) + EXP(- BUNKEL))
C      IF(AK2 * TIME .LE. 1.0E-10) AK2 = 1.0E-10/TIME
C      F        = (1.0 - ((1.0 - AK1) * ((1.0 - EXP(-AK2 * TIME))/(AK2 *
=      TIME )))

```

TABLE A-12.II (continued)

```

C      IF (F .GT. 1.0) F = 1.0
      IF (F .LE. 0.0) F = 0.0
C
      FMA      = F * FMGPR(L) + CC2(L) * (1.0 - EXP(-AK2 * TIME))
      IF (GBBG(L) .LE. 0.0) GBBG(L) = FMA / 1000000.0
      GBBG(L) = GBBG(L) + FMA
C
C      FISSION GAS WHICH IS NOT RELEASED FROM THE GRAIN BOUNDARY IS
C      LABELED GBBG(L)
C
C      CALCULATION OF GRAIN BOUNDARY GAS RELEASE
C
      DEN      = FDENS / 10970.0
      FP       = 1.0 - DEN
      P        = 1.0 / (1.0 + (1.0 / FP - 1.0) * 1.0E 05 / (GRNSIZ(L) ** 3.0))
      FBR      = (1.0 - ERF(P)) * EXP(-BUNKEL)
      IF (FTEMP .GT. 2100.0) FBR = 1.0 - (1.0 - FBR) / (FTEMP - 2100.)
      IF (FBR .LE. 0.0) FBR = 0.0
      IF (FBR .GT. 1.0) FBR = 1.0
C
      FMAA     = FBR * GBBG(L)
      GBBG(L) = GBBG(L) - FMAA
      FMGR(L) = FMGR(L) + FMAA
      CC2(L)  = CC2(L) + FMGPR(L) - FMA
C
      RETURN
      END

```

TABLE A-12.III

FGASRL UPDATE FOR FRAP-S3

(Used to Compare FGASRL Predictions with Experimental Gas Release Data)

```

4,FGMGP, F, GNSIZ, BP)                                MAIN2960
4,FMGP, F, GNSIZ, BP)                                FGRL0100
4,HMGP(21,2),GBBG(11,16),FMAA(11) , GNSIZ(16,11)     FGRL0240
ERF(X) = 1.0 - 0.348024 * 1.0/(1.0 + 0.47047 * X) +   FGRL0941
= 0.0958798 * (1.0/(1.0 + 0.47047 * X)) **2.0 -
= 0.7478556 * (1.0/(1.0 + 0.47047 * X)) ** 3.0 + 0.000025
$DELETE FGRL2280
IF(IT .EQ. 1) GBBG(L,J) = 0.0                        FGRL2281
IF(IT .EQ. 1) FMAA(L) = 0.0
TT = TFR(L - 1)
IF (L .LE. 1) TT = TFR(L)
TA = ((TFR(L) - TT)/2.0 + TT - 32.0)*5.0/9.0 + 273.16
IF(BP .LE. 0.0) BP = 1.0
BUNKEL = 1.25E14/(BP**3.0)
IF(BUNKEL .GE. 460.0) BUNKEL = 400.0
AK1(L) = 9.0E 07 * (EXP(-45289.86/TA)) + 0.0005      FGRL2320
AK2(L) = 0.00005* AK1(L) * (1.0 - 1.0/(EXP((TA - 1900.)/40.))
= + 1.0) + EXP(- BUNKEL)) * 3600.                  FGRL2340
IF(AK2(L) * DELH .LE. 1.0E-10) AK2(L) = 1.0E-10/DELH FGRL2341

C
G = GNSIZ(J,L)
IF(G .EQ. 0.0) G = 5.0
FP = 1. - DEN/ 100.
P = 1.0/(1.0 + (1.0/FP - 1.0) * 1.0E05 / (G**3.0))
FBR = (1.0 - ERF(P )) + EXP(-BUNKEL)
IF(TA .GE. 2100.) FBR = 1.0 - (((1.0 -FBR)/(TA - 2100.))
IF(FBR .GT. 1.0) FBR = 1.0

C
C FISSION GAS WHICH IS NOT RELEASED FROM THE GPAIN BOUNDARY IS
C LABELED GBBG(L,J)
C
$DELETE FGRL2560
$DELETE FGRL2580
FMA(L) = F(L,I) * FMGPR(L) + CC1(L,J) *(1.0 - EXP(-AK2(L) *
= DELH))                                             FGRL2560
IF(GBBG(L,J) .LE. 0.0) GBBG(L,J) = FMA(L) / 10000000. FGRL2580
GBBG(L,J) = GBBG(L,J) + FMA(L)                      FGRL2601
FMAA(L) = FBR * GBBG(L,J)
GBBG(L,J) = GBBG(L,J) - FMAA(L)
FMGR(J,I) = FMGR(J,I) + FMAA(L)
$DELETE FGRL2640

```

12.5 REFERENCES

- A-12.1 D. R. Coleman, E. T. Laats, N. R. Scofield, FRAP-S3: A Computer Code for Steady-State Analysis of Oxide Fuel Rods, Volume 2, Model Verification Report, TFBP-TR-228 (August 1977).
- A-12.2 J. Weisman, P. E. MacDonald, et al, "Fission Gas Release from UO_2 Fuel Rods with Time Varying Power Histories," Transactions of the American Nuclear Society, 12 (1969) pp 900-901.
- A-12.3 R. Souhler, "Fission-Gas Release from UO_2 During Irradiation up to 2,000°C," Nuclear Applications, 2 (April 1966).
- A-12.4 M. R. Hayns and M. H. Wood, "Models of Fission Gas Behavior in Fast Reactor Fuels Under Steady State and Transient Conditions," Journal of Nuclear Materials, 67 (1977) pp 155-170.
- A-12.5 R. M. Carroll, et al, "Fission Density, Burnup, and Temperature Effects on Fission-Gas Release From UO_2 ," Nuclear Science and Engineering, 38 (1969) pp 143-155.
- A-12.6 R. M. Carroll, "Fission-Gas Behavior in Fuel Materials," Nuclear Safety, 8 No. 4 (Summer 1967) pp 345-353.
- A-12.7 R. M. Carroll and O. Sisman, "In-Pile Fission-Gas Release from Single Crystal UO_2 ," Nuclear Science and Engineering, 21 (1965) pp 147-158.
- A-12.8 J. A. Turnbull, "The Mobility of Intragranular Bubbles in Uranium Dioxide During Irradiation," Journal of Nuclear Materials, 62 (1976) pp 325-328.
- A-12.9 D. Stahl and T. J. Partrician, Fission-Gas Behavior During A Mild Over-Power Transients, ANL 8069 (February 1974).
- A-12.10 C. J. Baroch and M. A. Rigdon, "Irradiation Behavior of UO_2 Burnups from 10 to 80 Gwd/tonne U," Paper No. 58, Proceedings of the BNES International Conference on Nuclear Fuel Performance, 15-19 October 1973, London (CONF-731004).
- A-12.11 A. D. Whapham, "Electron Observation of the Fission-Gas Bubble Distribution in UO_2 ," Nuclear Applications, 2, (1966).
- A-12.12 W. Beere and G. L. Reynolds, "The Morphology and Growth Rate of Interlinked Porosity in Irradiated UO_2 ," Journal of Nuclear Materials, 47 (1973) pp 51-57.
- A-12.13 D. R. Olander, Fundamental Aspects of Nuclear Reactor Fuel Elements, U. S. Department of Commerce, Springfield, Virginia, TID - 26711-P1 (1976).
- A-12.14 L. R. Kelman, Transient Fuel Response and Fission-Product Release Program - Quarterly Progress Report, ANL-75-72 (July - September 1975).

- A-12.15 R. B. Poeppel, "An Advanced Gas Release and Swelling Sub-routine," Proceedings of the ANS Conference on Fast Reactor Fuel Element Technology, Hinsdale, Ill., 1976, pp 311-326.
- A-12.16 J. A. Turnbull, "The Effect of Grain Size on the Swelling and Gas Release Properties of UO_2 During Irradiation," Journal of Nuclear Materials, 50 (1974) pp 380-391.
- A-12.17 R. G. Sachs and J. A. Kyger, Light-Water-Reactor Safety Research Program: Quarterly Progress Report, ANL-77-59 (April-June 1977).
- A-12.18 S. L. Seiffert, Power-Cooling-Mismatch Test Series Test PCM-3 Postirradiation Examination, TREE-NUREG-1187 (December 1977).
- A-12.19 J. A. Dearien and G. A. Berna, et al, FRAP-S3: Analytical Models and Input Manual - FRAP-S3: A Computer Code for the Steady-State Analysis of Oxide Fuel Rods - Volume 1, TFBP-TR-164 (October 1977).
- A-12.20 M. J. F. Notley and J. R. MacEwan, The Effect of UO_2 Density of Fission Product Gas Release and Sheath Expansion, Report AECL-2230 (1965).
- A-12.21 M. J. F. Notley, et al, Zircaloy Sheathed UO_2 Fuel Elements Irradiated at Values of $\dot{q}$ Between 40 and 83 W/cm, AECL-1676 (December 1962).
- A-12.22 C. E. Beyer and C. R. Hann, Prediction of Fission Gas Release from UO_2 Fuel, BNWL-1875, Battelle Northwest Laboratories (November 1974).
- A-12.23 W. R. Smalley, Saxton Core II Fuel Performance Evaluation Part I: Materials, WCAP-3385-56, Part I (September 1971).
- A-12.24 R. G. Bellamy and Rich, Grain-Boundary, Gas Release in High Burn-up Uranium Dioxide, Journal of Nuclear Materials 33 (1969).
- A-12.25 W. R. Smalley, Evaluation of Saxton Core III Fuel Materials Performance, WCAP-3385-57 (1974).
- A-12.26 K. Taketani and M. Ichikawa, "Fuel Irradiation Experiments by JAERI for Light Water Reactors," Contribution to Crest Specialist Meeting, Sacley, France, October 21-24, 1973.
- A-12.27 W. E. Bailey et al, "Effect of Temperature and Burnup on Fission-Gas Release in Mixed Oxide Fuel," Journal of the American Ceramic Society, 49 (1970).

- A-12.28 I. Devold, A Study of the Temperature Distribution in UO₂ Reactor Fuel Elements, AE-318 (1968).
- A-12.29 M. F. Lyons et al, UO₂ Fuel Rod Operation with Gross Central Melting, GEAP-4262 (1963).
- A-12.30 R. M. Berman et al, Irradiation Behavior of Zircaloy-Clad Fuel Rods Containing Dished End UO₂ Pellets, WAPD-TM-629 (July 1967).
- A-12.31 J. T. Engle and H. B. Meieran, Performance of Fuel Rods Having 97 Percent Theoretical Density UO₂ Pellets Sheathed in Zircaloy-4 and Irradiated at Low Thermal Ratings, WAPD-TM-631 (July 1968).
- A-12.32 N. Fuhrman et al, Evaluation of Fuel Rod Performance in Maine Yankee Core I, Task C, EPRI-NP-218 (November 1976).
- A-12.33 Light-Water-Reactor Safety Research Program: Quarterly Progress Report, April - June 1975, ANL-75-58 (June 1975).
- A-12.34 Jean-Claude Janvier et al, Irradiation of Uranium Dioxide in a Resistant Cladding Effects of Initial Diametral Gap on Overall Behavior, CEA-R-3358 (October 1967).
- A-12.35 J. P. Stora and P. Chenebault, Programme Cyrano-Mesure de l'integrale de conductibilite thermique d' UO₂ fritte jusqu'a 2,300°C - Evolution des gaz de fission a puissance constante, CEA-R-3618 (1968).
- A-12.36 R. D. MacDonald and A. S. Bain, Irradiation of Zircaloy-2 Clad UO₂ to Study Sheath Deformation, AECL-1685 (1962).
- A-12.37 M. D. Freshly, "Mixed-Oxide Fuel Irradiations in the Plutonium Recycle Test Reactor," Nuclear Technology, 15 (August 1972), pp. 138, 141, 169, 172-3.
- A-12.38 F. H. Megerth et al, Zircaloy-Clad UO₂ Fuel Rod Evaluation Program, GEAP-10371 (June 1971).
- A-12.39 T. B. Burley and M. D. Freshley, "Internal Gas Pressure Behavior in Mixed-Oxide Fuel Rods During Irradiation," Nuclear Applications and Technology, 9 (August 1970).
- A-12.40 M. J. F. Notley, R. Deshaies, et al, Measurements of the Fission Product Gas Pressures Developed in UO₂ Fuel Elements During Operation, AECL-2662 (1966).
- A-12.41 E. De Meulemeester et al, "Review of Work Carried out by BELGONCLEAIRE and CEA on the Improvement and Verification of the Computer Code with the Aid of In-Pile Experimental Results," British Nuclear Energy Society International Conference on Nuclear Fuel Performance, October 15-19, 1973.
- A-12.42 R. M. Carroll, "Fission Product Release from UO₂," Nuclear Safety, 4(1) (1962).