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SAND2013-3906
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Printed May 2013

Sensitivity Analysis of the Fission Gas Behavior Model in BISON

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Sensitivity Analysis of the Fission Gas Behavior Model in BISON

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Abstract

This report summarizes the result of a NEAMS project focused on sensitivity analysis of a new model for the fission gas behavior (release and swelling) in the BISON fuel performance code of Idaho National Laboratory. Using the new model in BISON, the sensitivity of the calculated fission gas release and swelling to the involved parameters and the associated uncertainties is investigated. The study results in a quantitative assessment of the role of intrinsic uncertainties in the analysis of fission gas behavior in nuclear fuel.

Acknowledgments

This work was funded by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program under the Advanced Modeling and Simulation Office (AMSO) in the Nuclear Energy Office in the U.S. Department of Energy. The authors specifically acknowledge the Program Manager of the Fuels Product Line, Dr. Steven Hayes (INL), and Dr. Keith Bradley, National Technical Director of NEAMS, for their support of this work. Finally, we thank the BISON and MOOSE development teams.

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Chapter 1

Introduction

This report summarizes the result of a NEAMS project focused on sensitivity analysis of a new fission gas behavior model in the BISON fuel performance code. BISON is an implicit, parallel, fully-coupled code under development at the Idaho National Laboratory (INL) (1). BISON is built on the MOOSE computational framework (2) which allows for rapid development of codes involving the solution of partial differential equations using the finite element method.

Nuclear fuel operates in an environment with complex multiphysics phenomena, occurring over distances ranging from inter-atomic spacing to meters, and times scales ranging from microseconds to years. This multiphysics behavior is often tightly coupled and many important aspects are inherently multidimensional. Most current fuel modeling codes employ loose multiphysics coupling and are restricted to 2D axisymmetric or 1.5D approximations (4; 5; 6). BISON is able to simulate tightly coupled multiphysics and multiscale fuel behavior, for either 2D axisymmetric or 3D geometries. Although the primary development focus thus far has been on simulating light water reactor fuel rods, BISON has also been applied to TRISO particle fuel in high temperature gas reactors and metallic fuel in both rod or plate form (1; 8). BISON code validation and assessment is presented in (3).

Among the various issues involved in nuclear fuel modeling, the processes induced by the generation of the fission gases xenon and krypton in nuclear fuel have a strong impact on the thermo-mechanical performance of the fuel rods. On the one hand, the fission gases tend to precipitate into bubbles resulting in fuel swelling, which promotes pellet-cladding gap closure and the ensuing pellet-cladding mechanical interaction (PCMI). On the other hand, fission gas release (FGR) to the fuel rod free volume causes pressure build-up and thermal conductivity degradation of the rod filling gas. Consequently, the fuel temperature increases, which in turn may lead to higher FGR (*thermal feedback*) until the rod fails due to cladding ballooning and cladding burst. Given the nature of fission gas release and swelling as potential fuel rod life-limiting factors, the reliable modeling of fission gas behavior is a primary requisite for fuel performance codes.

The inherently coupled kinetics of the fission gas release and swelling calls for the development of physics-based models of these phenomena to be employed in the fuel performance codes. As of today, however, empirical approaches are often adopted. These models are efficient to use but unfit for providing insight into the underlying mechanisms, and cannot be applied beyond their range of calibration. Recently, a new physics-based model of fission gas release and swelling in UO_2 was incorporated in the BISON fuel performance code. The new model is based on the approach

described in (10), and practically combines a physical description of the relevant mechanisms with a level of simplicity suitable for the effective application to engineering-scale nuclear fuel analysis. The model incorporates the fundamental features of fission gas behavior, among which are gas generation, diffusion and precipitation in grains, growth and coalescence of gas bubbles at grain faces, grain growth and grain boundary sweeping, thermal, athermal, and transient gas release. Compared to the models previously adopted in BISON, the new model allows calculating the fission gas release and swelling as inherently coupled processes, also introducing the flexibility and the accuracy of a physics-based treatment in contrast with empirical approaches.

It is well known that the uncertainties pertaining to some parameters like the gas atom diffusion coefficient significantly affect the accuracy of fission gas behavior calculations (e.g., (10; 11; 12)). In order to assess the sensitivity of the calculated fission gas release and swelling to the basic parameters, and to better quantify the impact of intrinsic uncertainties on the predictions of current fission gas behavior models, a sensitivity analysis is carried out in this work using the new model in the BISON code.

The outline of the report is as follows: Chapter 2 discusses the input parameters chosen for the sensitivity analysis, Chapter 3 describes the software framework that enabled this sensitivity analysis (specifically, the integration of the DAKOTA code with BISON), Chapter 4 presents results, and Chapter 5 provides a summary.

Chapter 2

Input Parameters for FGR Model

The input parameters we considered for the sensitivity analysis were:

- Linear heat rate. This parameter describes the linear power of the fuel. It determines the temperature in the fuel, which strongly affects the fission gas behavior through the gas diffusion coefficient (see below) and the equation of state of the gas in the bubbles.
- Gas diffusion coefficient. The first and basic step in fission gas behavior is gas diffusion from within the fuel grains to the grain faces, which is controlled by the diffusion coefficient of gas atoms in the UO_2 lattice. The diffusion coefficient presents an exponential dependence on temperature, and is subject to considerable uncertainty (at least a factor of 10 (11; 12)), which limits the predictive accuracy achievable by fission gas behavior models.
- UO_2 /gas specific surface energy. This parameter determines the surface tension of grain-face gas bubbles and affects the kinetics of bubble growth, and consequently of fission gas release and swelling.
- Hydrostatic pressure. This parameter describes the hydrostatic pressure acting on the gas bubbles, which – along with the bubble surface tension – affects the kinetics of bubble growth.
- Fuel Grain Radius. Grain size affects the rate of gas diffusion from within the fuel grains to the grain faces through the relevant diffusion equation.
- Grain boundary sweeping model. This model may be turned on or off. When on, the model considers the additional contribution to gas accumulation at grain faces due to gas sweeping by moving grain boundaries as the grain growth process takes place.
- Fuel porosity. Porosity affects the fuel thermal conductivity and temperature, and consequently the fission gas behavior (see above).

Chapter 3

Software Framework

To perform the sensitivity analysis, we interfaced a toolkit called DAKOTA to the BISON fuel performance code on the High Performance Computing (HPC) machine called fission at Idaho National Laboratory. DAKOTA allows a user to design computer experiments, run parameter studies, perform uncertainty quantification, and calibrate parameters governing their simulation model. A primary goal for DAKOTA is to provide scientists and engineers with a systematic and rapid means to obtain improved or optimal designs or understand sensitivity or uncertainty using simulation-based models. These capabilities generally lead to improved designs and better understanding of system performance (7).

One of the primary advantages that DAKOTA has to offer is access to a broad range of iterative capabilities through a single, relatively simple interface between DAKOTA and a simulator. In this context, we interfaced DAKOTA to BISON. To perform different types of analyses, it is only necessary to change a few commands in the DAKOTA input and start a new analysis. The need to learn a completely different style of command syntax and the need to construct a new interface each time you want to use a new algorithm are eliminated. For the work presented below, we were able to develop one interface between DAKOTA and BISON, and swap out a few lines in the DAKOTA input deck to run the various case studies.

There are many goals of running a computer experiment: one may want to explore the input domain or the design space and get a better understanding of the range in the outputs for a particular domain. Another objective is to determine which inputs have the most influence on the output, or how changes in the inputs change the output. This is usually called *sensitivity analysis*. In contrast, *uncertainty quantification (UQ)* refers to taking a particular set of distributions on the inputs, and propagating them through the model to obtain a distribution on the outputs. Typically, structured experimental designs are used for sensitivity analysis. These methods, such as the design and analysis of computer experiments (DACE) methods, are techniques which seek to extract as much trend data from a parameter space as possible using a limited number of sample points. Space filling designs such as orthogonal array sampling and Latin Hypercube sampling are commonly used for sensitivity analysis. Note that Latin Hypercube Sampling may also be used for UQ. In the context we present, we assume the input parameters are uniformly distributed when using LHS, and the main focus is sensitivity analysis.

The studies we ran to perform sensitivity analysis involved two types:

- **Orthogonal Array Sampling (OAS).** In orthogonal arrays, the input parameters are specified at fixed levels (e.g. low, medium, high), and the OAS design is constructed so that the sample columns (e.g. columns for particular parameter settings) are orthogonal to each other. We used a full factorial orthogonal array for these studies, which means we considered the full tensor product of all the combinations of parameter levels. Orthogonal arrays allow one to perform main effects analysis. This is a sensitivity analysis method which identifies the input variables that have the most influence on the output. In main effects, the idea is to look at the mean of the response function when variable A (for example) is at level 1 vs. when variable A is at level 2 or level 3. If these mean responses of the output are statistically significantly different at different levels of variable A, this is an indication that variable A has a significant effect on the response. The orthogonality of the columns is critical in performing main effects analysis, since the column orthogonality means that the effects of the other variables 'cancel out' when looking at the overall effect from one variable at its different levels.
- **Latin Hypercube Sampling (LHS).** Latin Hypercube sampling is a stratified sampling technique for which the range of each uncertain variable is divided into N_s segments of equal probability, where N_s is the number of samples requested. The relative lengths of the segments are determined by the nature of the specified probability distribution (e.g., uniform has segments of equal width, normal has small segments near the mean and larger segments in the tails). For each of the uncertain variables, a sample is selected randomly from each of these equal probability segments. These N_s values for each of the individual parameters are then combined in a shuffling operation to create a set of N_s parameter vectors with a specified correlation structure. A feature of the resulting sample set is that *every row and column in the hypercube of partitions has exactly one sample*. Since the total number of samples is exactly equal to the number of partitions used for each uncertain variable, an arbitrary number of desired samples is easily accommodated (as compared to less flexible approaches in which the total number of samples is a product or exponential function of the number of intervals for each variable, i.e., many classical design of experiments methods).

LHS techniques, in general, require fewer samples than traditional Monte Carlo for the same accuracy in statistics, but they still can be prohibitively expensive. For further information on the method and its relationship to other sampling techniques, one is referred to Helton and Davis (14). Note that under certain separability conditions associated with the function to be sampled, Latin hypercube sampling provides a more accurate estimate of the mean value than does random sampling. That is, given an equal number of samples, the LHS estimate of the mean will have less variance than the mean value obtained through random sampling.

Figure 3.1 demonstrates Latin hypercube sampling on a two-variable parameter space. Here, the range of both parameters, x_1 and x_2 , is $[0, 1]$. Also, for this example both x_1 and x_2 have uniform statistical distributions. For Latin hypercube sampling, the range of each parameter is divided into p "bins" of equal probability. For parameters with uniform distributions, this corresponds to partitions of equal size. For n design parameters, this partitioning yields a total of p^n bins in the parameter space. Next, p samples are randomly selected in the parameter space, with the following restrictions: (a) each sample is randomly placed inside a bin, and (b) for all one-dimensional projections of the p samples and bins, there will be

one and only one sample in each bin. In a two-dimensional example such as that shown in Figure 3.1, these LHS rules guarantee that only one bin can be selected in each row and column. For $p = 4$, there are four partitions in both x_1 and x_2 . This gives a total of 16 bins, of which four will be chosen according to the criteria described above. Note that there is more than one possible arrangement of bins that meet the LHS criteria. The dots in Figure 3.1 represent the four sample sites in this example, where each sample is randomly located in its bin. There is no restriction on the number of bins in the range of each parameter, however, all parameters must have the same number of bins.

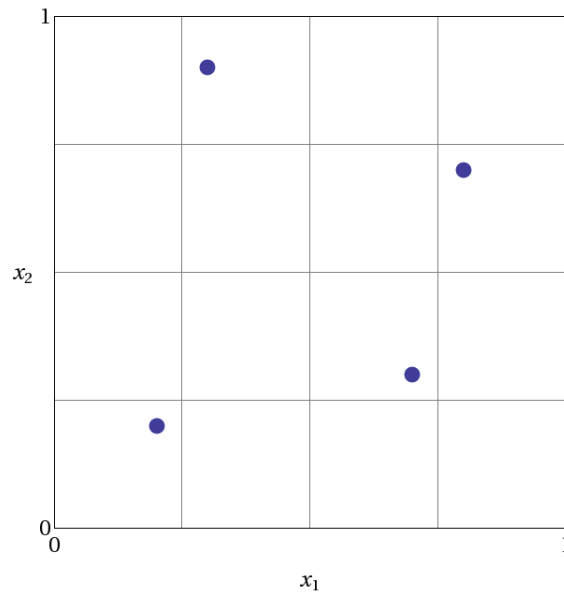


Figure 3.1. An example of Latin hypercube sampling with four bins in design parameters x_1 and x_2 . The dots are the sample sites.

Chapter 4

Results

4.1 Initial LHS Studies

The first analysis we performed was a Latin Hypercube sampling over all seven parameters, with the values and/or bounds given in Table 4.1. We considered a simple 2D, single-pellet problem. 200 LHS samples were generated. A scatterplot matrix of these samples is shown in Figure 4.1. Note that, in order to study the impact of the uncertainties pertaining to the gas diffusion coefficient, the sensitivity study on this parameter involved multiplications by factors of 1/5 and 5. The gas diffusion coefficient itself is dependent on temperature. Fuel porosity is also a dimensionless quantity, with values between 0 and 1. The other parameters' dimensions are given in the table.

Based on the upper row of the scatterplot matrix, we see that Linear Heat Rate is perfectly correlated with Rod Total Power, which is to be expected. We also see that the other parameters are not strongly correlated with Rod Total Power. The bottom row of the matrix shows scatterplots of the parameters with respect to the fraction of the fission gas released, which is defined as the amount of fission gas released divided by the amount of fission gas produced. There is no fission gas released until the linear heat rate is around 20,000 W/m. Then, LHR is strongly correlated to the fraction FGR. There is some correlation between the other input parameters and fraction FGR. The actual correlation coefficients are shown in Figure 4.2. Correlation coefficients have a value between -1 and 1. If the absolute value of the correlation coefficient is near one, we say there is a strong correlation. For example, Linear Heat Rate and Rod Total Power are perfectly

Table 4.1. Input Parameter Specification

Parameter	Lower Bound or Values	Upper Bound or Values
Linear Heat Rate (W/m)	25,000	45,000
Diffusion Coefficient Multiplier (-)	0.2, 1.0, and 5.0	
Hydrostatic Pressure (Pa)	0.0	100.E+6
Specific Surface Energy (J/m ²)	0.5	1.0
Fuel Grain Radius (m)	0.2E-6	15.0E-6
Fuel Porosity	0.0	0.1
Grain Boundary Sweeping Model	1 (off)	2 (on)

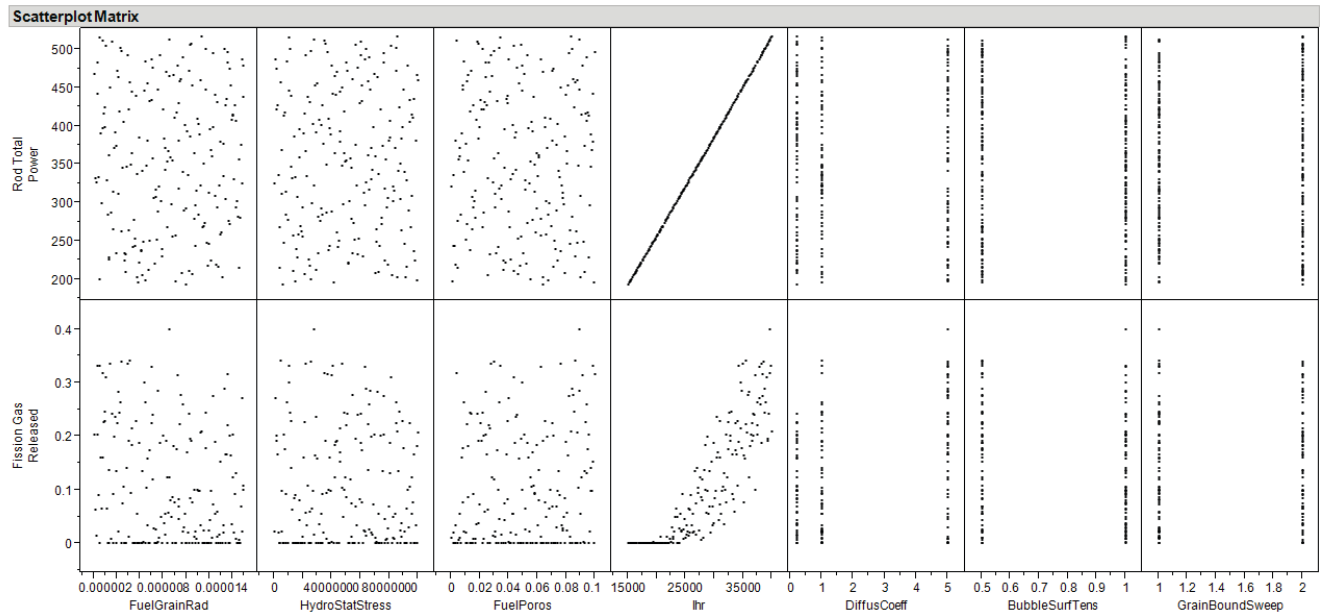


Figure 4.1. Scatterplot matrix based on 200 LHS samples over 7 input parameters

correlated: as LHR increases, so does Rod Total Power. If the correlation coefficient is zero, the variables are uncorrelated. Correlations are always calculated between two sets of sample data. The correlation coefficients presented in here are Pearson's correlation coefficient, which is defined for two variables x and y as:
$$\text{Corr}(x,y) = \frac{\sum_i(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_i(x_i - \bar{x})^2 \sum_i(y_i - \bar{y})^2}}$$
.

	<i>FuelGrainRad</i>	<i>HydroStatStress</i>	<i>FuelPoros</i>	<i>lhr</i>	<i>DiffusCoeff</i>	<i>BubbleSurfTens</i>	<i>GrainBoundSweep</i>
FuelGrainRad	1.000						
HydroStatStress	0.004	1.000					
FuelPoros	0.008	-0.002	1.000				
lhr	0.010	0.010	-0.014	1.000			
DiffusCoeff	-0.017	0.048	0.004	0.027	1.000		
BubbleSurfTens	0.014	-0.018	0.036	-0.037	0.038	1.000	
GrainBoundSweep	0.059	-0.080	-0.032	0.017	0.000	0.000	1.000
Rod Total Power	0.009	0.010	-0.014	1.000	0.027	-0.038	0.018
Fraction Fission Gas Released	-0.205	-0.049	0.132	0.868	0.280	-0.063	0.018

Figure 4.2. Correlation Coefficients between BISON Inputs and Outputs for the FGR model

The next analysis we performed was to focus on one value of Linear Heat Rate, because it was so dominant with respect to FGR: we wanted to control it and sample more extensively over the other parameters to better understand their effects. The results of this sampling (another 200 samples with LHR held fixed at 30,000 W/m) are shown in Figure 4.3 and Figure 4.4.

At a constant LHR, the correlations of the other parameters are stronger: the diffusion coefficient is the most strongly correlated with fraction Fission Gas Released, followed by Fuel Porosity and the negative correlation of Fuel Grain Radius to FGR.

	<i>FuelGrainRad</i>	<i>HydroStatStress</i>	<i>FuelPoros</i>	<i>DiffusCoeff</i>	<i>BubbleSurfTens</i>	<i>GrainBoundSweep</i>
FuelGrainRad	1.000					
HydroStatStress	-0.008	1.000				
FuelPoros	0.018	-0.016	1.000			
DiffusCoeff	0.009	-0.030	-0.002	1.000		
BubbleSurfTens	0.028	0.011	0.060	0.068	1.000	
GrainBoundSweep	-0.030	-0.030	-0.052	-0.015	0.060	1.000
Fraction Fission Gas Released	-0.354	-0.139	0.462	0.716	0.059	0.018

Figure 4.3. Correlation Coefficients between BISON Inputs and Outputs for the FGR model, with LHR = 30,000 W/m

The scatterplot is colored by the value of the diffusion coefficient. The samples with diffusion coefficient multiplier = 0.2 are colored in red, with diffusion coefficient multiplier = 1 in green, and with diffusion coefficient multiplier = 5 in black. One advantage of this is that one can better distinguish what is controlling the simulation behavior. For example, as expected the lowest value of diffusion coefficient tends to give lower FGR. You can see that not only on the fourth picture of DiffusCoeff vs. Fission Gas Released, but also on the first three pictures, especially the third with fuel porosity: at a particular fuel porosity, the samples with low diffusion coefficient give smaller FGR values than others.

The dominant role of the uncertainties pertaining to the diffusion coefficient in affecting the predictions of current fission gas behavior model appears to be confirmed by this study.

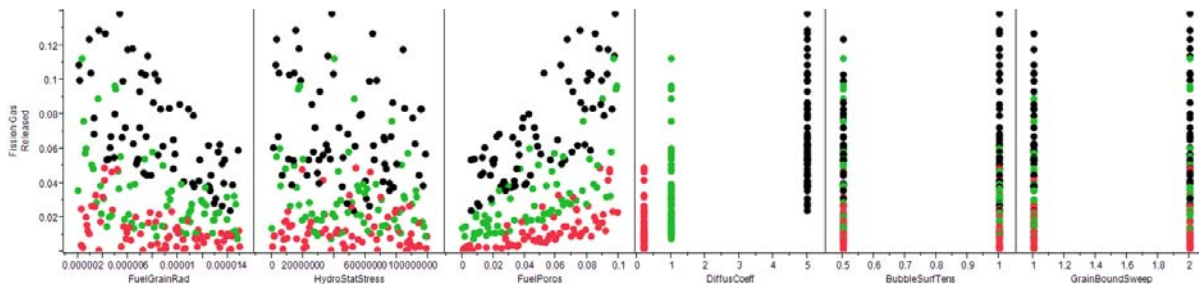


Figure 4.4. Scatterplot matrix based on 200 LHS samples over 6 input parameters, with LHR = 30,000 W/m. Red points have diffusion coefficient multiplier = 0.2, green points have diffusion coefficient multiplier = 1.0, black points have diffusion coefficient multiplier = 5.0

Table 4.2. Input Parameter Specification for Orthogonal Array

Parameter	Values
Linear Heat Rate (W/m)	25000, 30000, 35000, 40000, and 45000
Diffusion Coefficient Multiplier (-)	0.2, 0.5, 1, 2, 3, 4, and 5
Hydrostatic Pressure (Pa)	50.E+6
Fuel Grain Radius (m)	0.5E-6
Specific Surface Energy (J/m ²)	0.5
Fuel Porosity	0.05
Grain Boundary Sweeping Model	off

4.2 Orthogonal Array Study

The next analysis we performed was an orthogonal array study. The purpose of this study was to better quantify the impact of the uncertainties pertaining to the diffusion coefficient. The input parameter settings for the other variables were held at a nominal level: only the diffusion coefficient and LHR varied. The diffusion coefficient multiplier had values of 0.2, 0.5, 1, 2, 3, 4, and 5. The LHR varied from 25,000 W/m to 45,000 W/m in increments of 5,000 W/m. We did a full factorial study, covering all the combinations. Thus, the total number of parameter runs was seven times five, or 35 runs. The parameter values are shown in Table 4.2.

The main results are shown in Figure 4.5. Each dot on a main effects plot shows the mean response at the input value on the abscissa. For example, the left-most point on the DiffusCoeff main effects plot shows the average of the Fraction FGR for all the samples that had a diffusion coefficient multiplier of 0.2. These plots show that the average Fraction FGR increases both as a function of the diffusion coefficient and also as a function of linear heat rate. The effect is stronger for LHR. Boxplots of these results in Figure 4.6 show more detail.

To look at this data a bit differently, we plot Fraction FGR as a function of the Diffusion Coefficient, but color-coded by LHR. This is shown in Figure 4.7. We also plot the Fraction FGR as a function of Centerline temperature, which is constant for a particular LHR value. The plots point out the strong influence of diffusion coefficient and temperature on FGR.

In order to assess how the uncertainties pertaining to the diffusion coefficient reflect on uncertainties in the calculated FGR, a study is proposed here on the FGR variation factor. The variation factor is calculated as the deviation between the FGR values obtained by using the maximum and the minimum considered diffusion coefficient. At a fixed LHR, we calculated the variation factor as:

$$VariationFactor = \frac{maximumFGR - minimumFGR}{minimumFGR} \quad (4.1)$$

The variation factor is plotted as a function of LHR in Figure 4.8. The variation factor is also

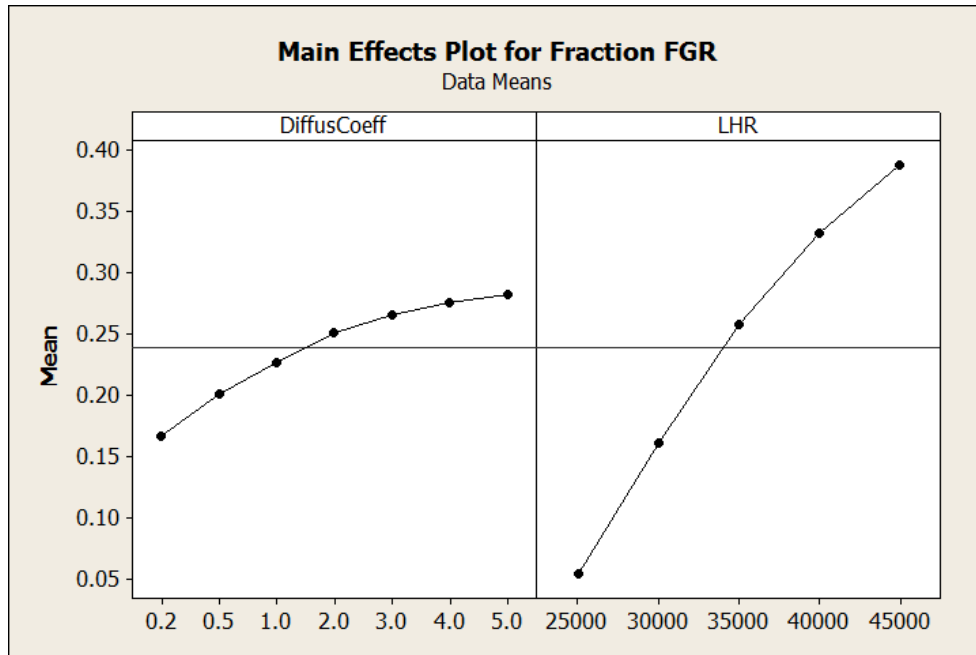


Figure 4.5. Main Effects Plot for Diffusion Coefficient Multiplier and for Linear Heat Rate, with respect to Fraction FGR

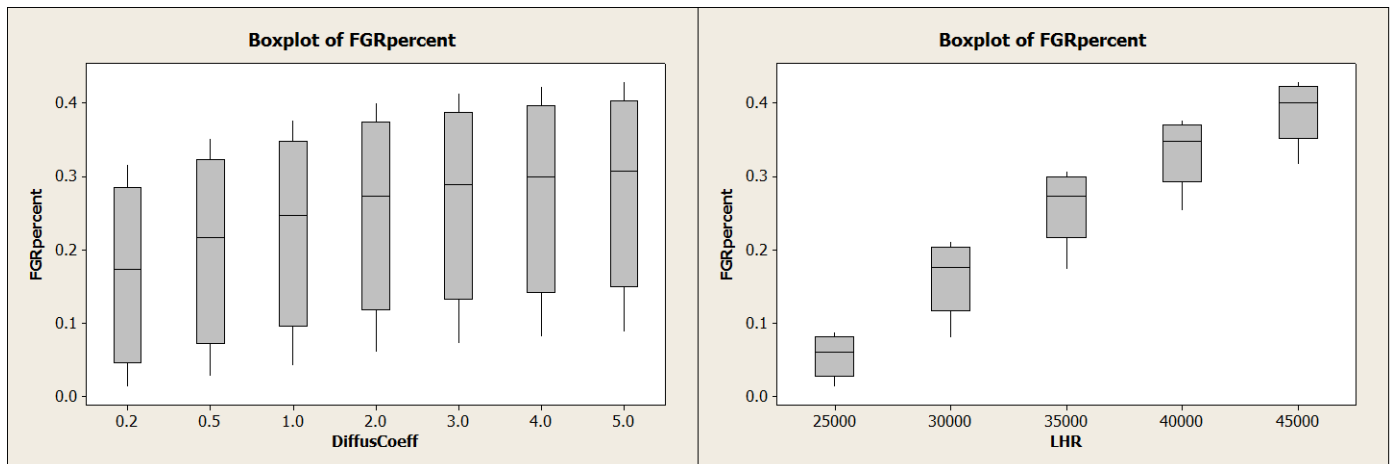


Figure 4.6. Boxplot of Results for Diffusion Coefficient Multiplier and Linear Heat Rate, with respect to Fraction FGR

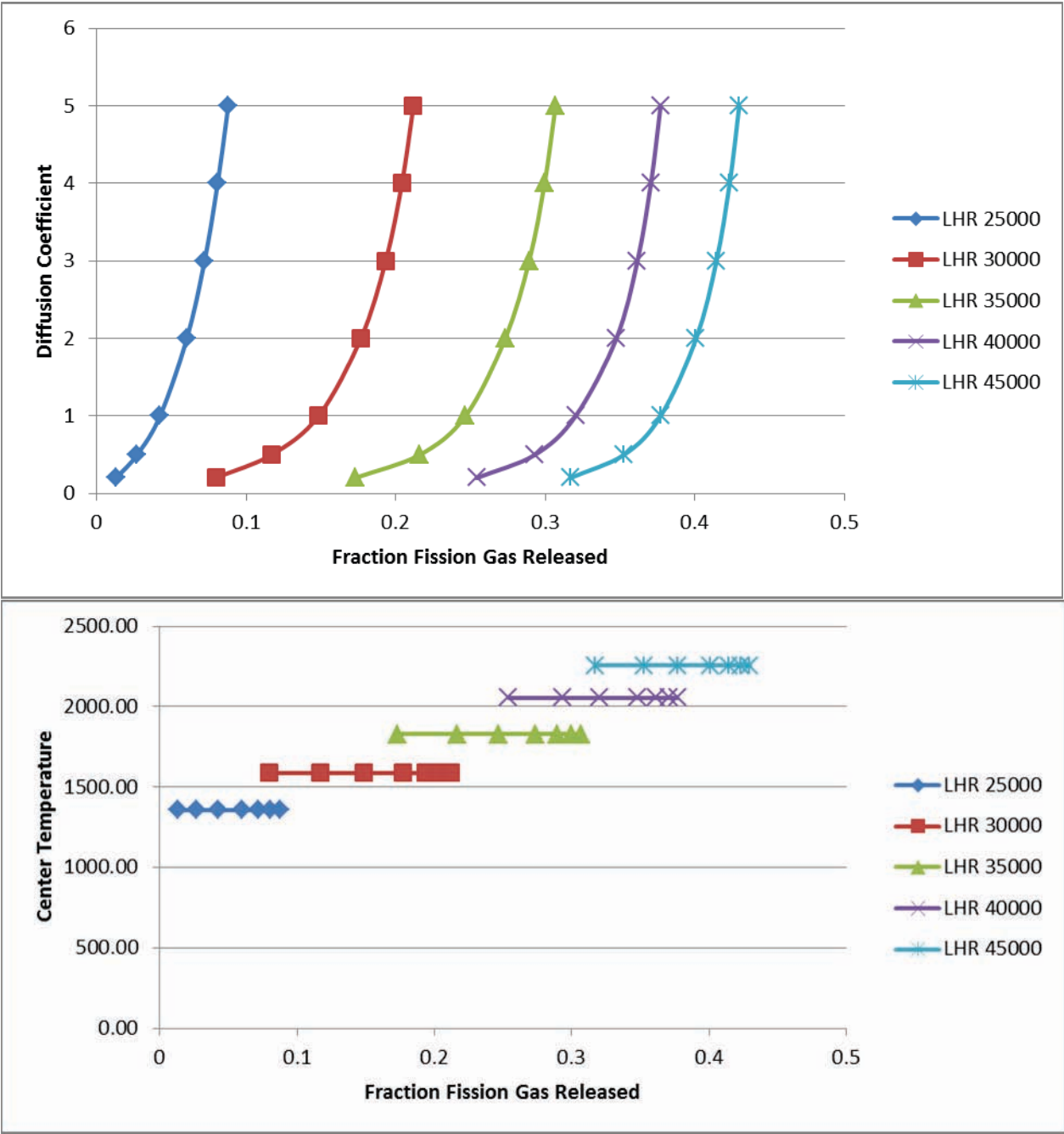


Figure 4.7. Fraction FGR as a function of Diffusion coefficient multiplier and LHR (top figure) and Fraction FGR as a function of Centerline Temperature and LHR (bottom).

plotted as a function of the Fraction FGR released at D multiplier = 1.

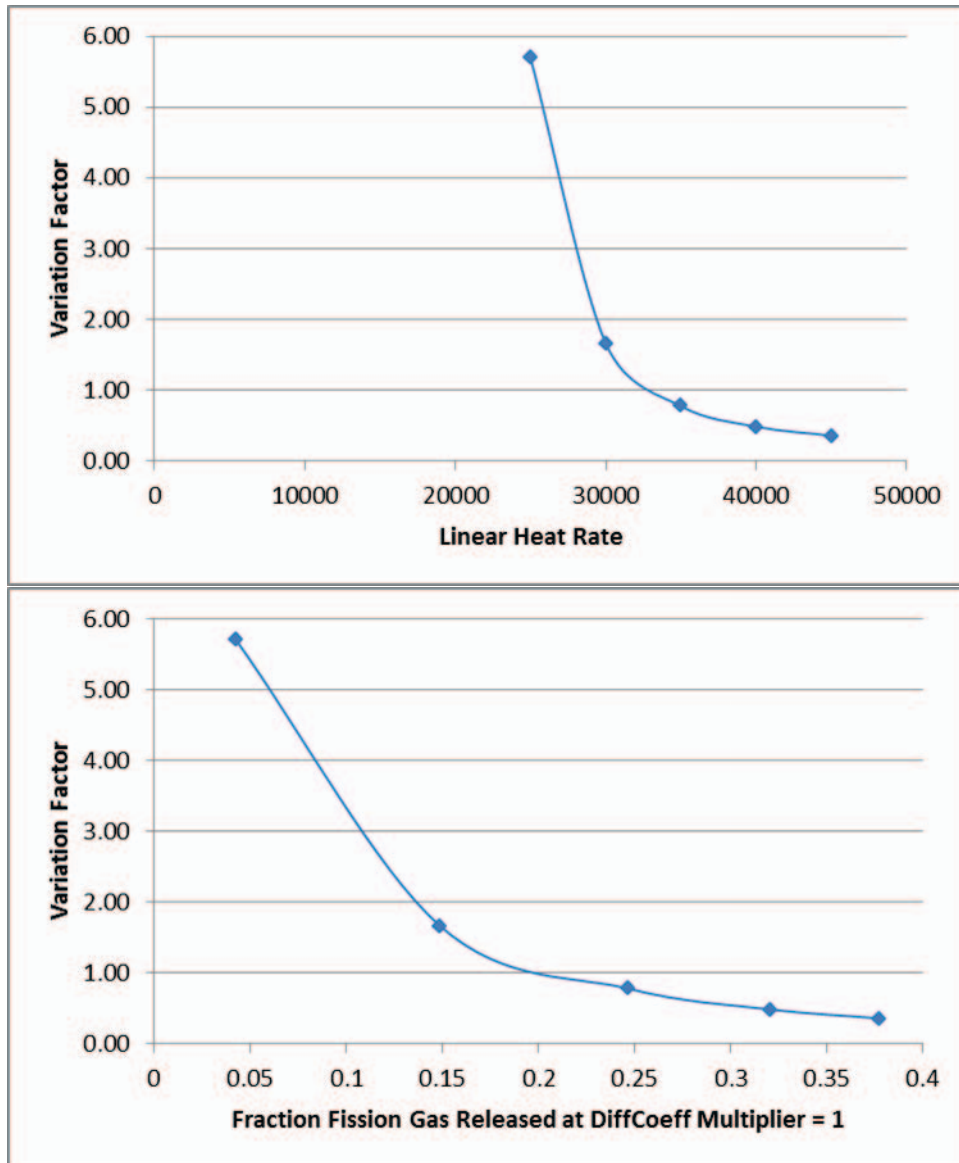


Figure 4.8. Variation Factor as a function of LHR (top figure) and as a function of Fraction FGR at D multiplier = 1 (bottom).

It can be noted that the variability in the fission gas diffusion coefficient can lead to a variation factor as high as 5-6 in the calculated FGR. This confirms that the discrepancies between FGR measurements and code calculations may be largely ascribed to the uncertainties pertaining to the diffusion coefficient. Moreover, the variation factor increases with decreasing FGR, which provides an explanation to the recognized difficulty to predict low FGR values (13) as brought about – at least to some degree – by the uncertainties pertaining to the diffusion coefficient.

4.3 Swelling

Finally, we examined the behavior of the model in terms of fission gas swelling. The current model of fission gas behavior in BISON is capable of analyzing both the fission gas release and swelling as inherently coupled processes. The previous analyses in this Chapter were all run with the swelling model off. We then ran the same orthogonal array study presented in the previous section with the parameters given in Table 4.2, but the swelling model was turned on. We examined the swelling with respect to three elements in the axial mid-plane, at the fuel center, mid pellet, and outer edge of the fuel.

Recall that the orthogonal array varied linear heat rate (LHR) and the Diffusion Coefficient multiplier. The main effects for these inputs with respect to the calculated fission gas swelling at the fuel center, mid-pellet, and the outer edge of the fuel are shown in Figures 4.9, 4.10, and 4.11. Note that the magnitude of the swelling is greatest in the fuel center, decreasing in the mid-pellet, and smallest at the outer edge. In all of these element locations, both linear heat rate and the diffusion coefficient multiplier have a positive correlation with swelling: swelling increases as these inputs are increased. Both effects are expected since (i) higher LHR means higher temperature, which results in larger fission gas bubbles in the fuel (through enhanced diffusion of gas atoms and through the equation of state of the gas in the bubbles) that induce higher swelling, and (ii) higher diffusion coefficient directly results in enhanced diffusion of gas atoms to the bubbles and hence larger bubbles size. Finally, we plotted the variation factor for swelling, defined by the following equation for a given LHR:

$$VariationFactor = \frac{maximumswelling - minimumswelling}{minimumswelling} \quad (4.2)$$

This is shown in Figure 4.12. The variation factor for swelling is greatest at smaller values of LHR. It is also has larger magnitude for the outer edge element. This is partly due to the small values of swelling at the outer edge, which show greater relative change. These results point out the significant impact of the uncertainties pertaining to the diffusion coefficient on the calculated fission gas swelling.

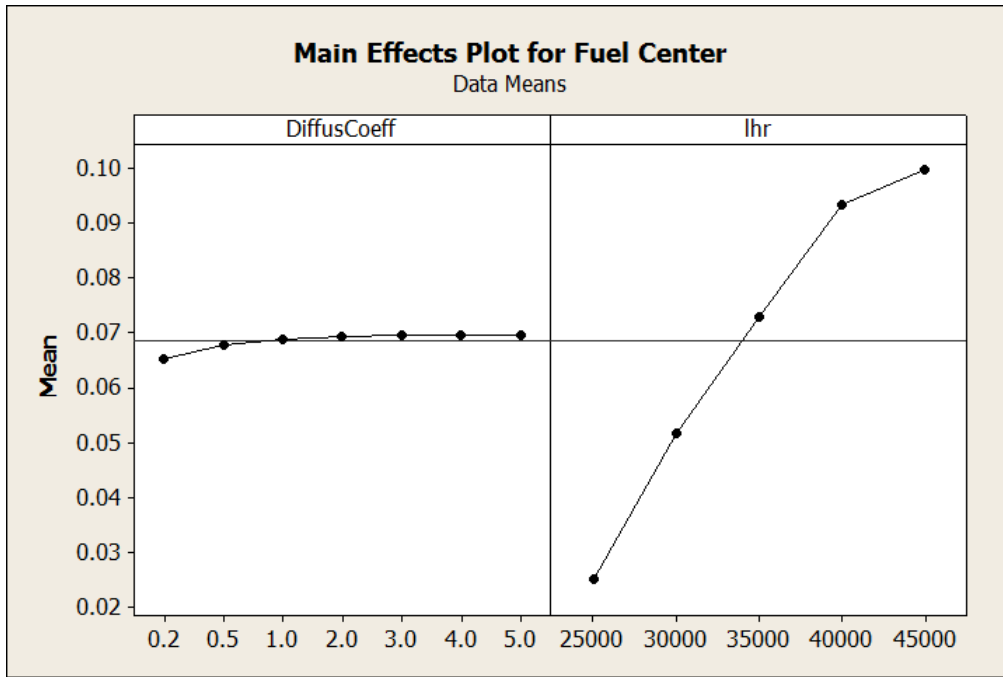


Figure 4.9. Main Effects Plot for Diffusion Coefficient Multiplier and Linear Heat Rate, with respect to Swelling at Fuel Center.

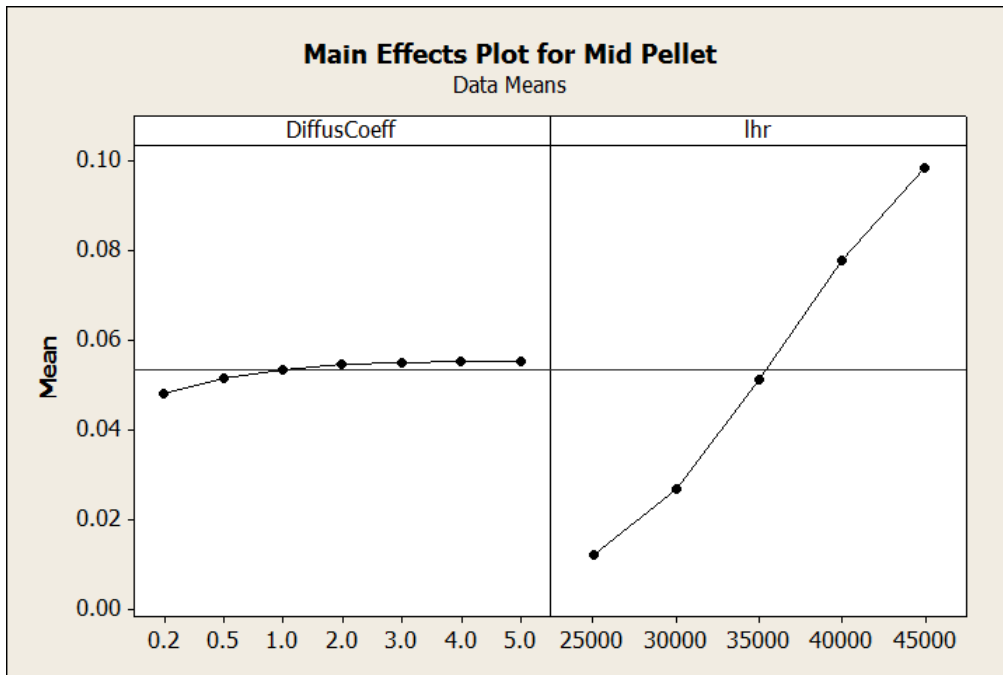


Figure 4.10. Main Effects Plot for Diffusion Coefficient Multiplier and Linear Heat Rate, with respect to Swelling at Mid Pellet.

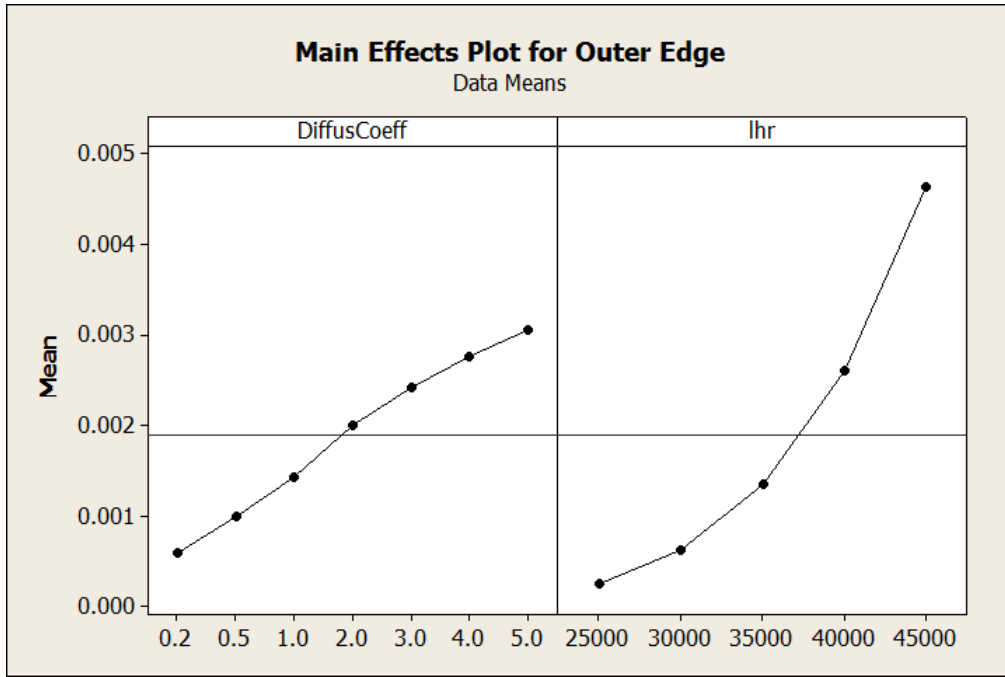


Figure 4.11. Main Effects Plot for Diffusion Coefficient Multiplier and Linear Heat Rate, with respect to Swelling at Outer Edge.

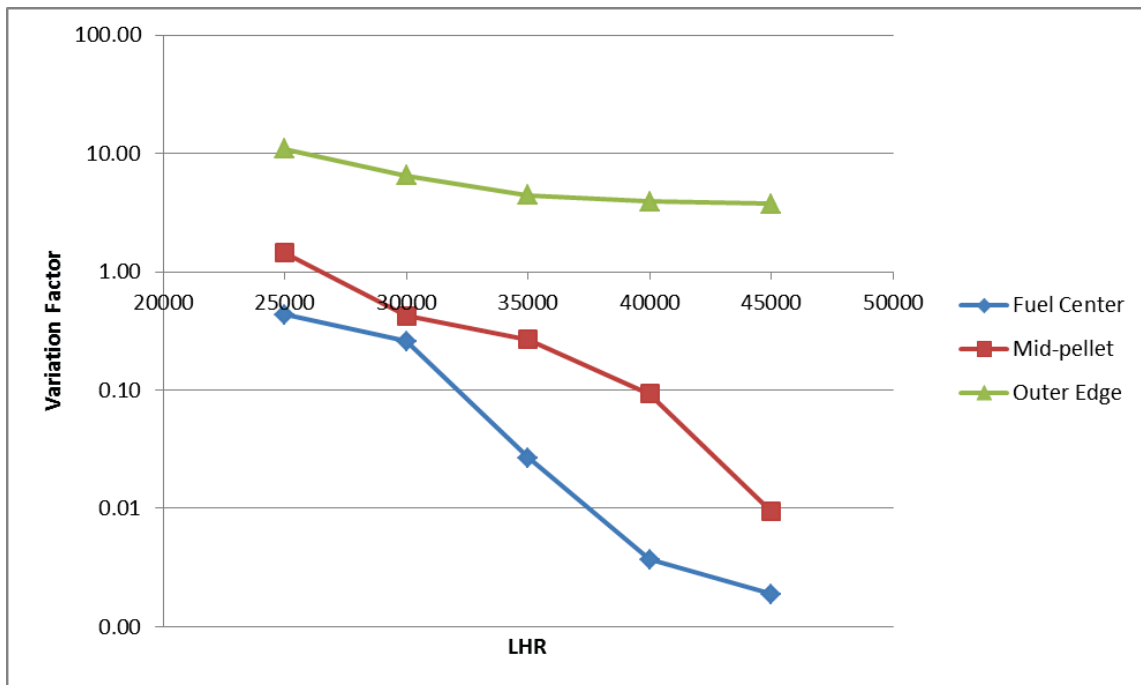


Figure 4.12. Variation Factor for Swelling as a function of Linear Heat Rate.

Chapter 5

Summary

This report summarizes the result of a NEAMS project focused on sensitivity analysis of a new model for the fission gas behavior (release and swelling) in the BISON fuel performance code of Idaho National Laboratory. Using the new model in BISON, the sensitivity of the calculated fission gas release and swelling with respect to several parameters was investigated.

Using a Latin Hypercube sampling study, we found that the fraction of Fission Gas Released was strongly correlated with the linear heat rate and the diffusion coefficient multiplier. It was also correlated, though less strongly, with the fuel grain radius and the fuel porosity. It was not highly correlated with the hydrostatic pressure or the bubble surface tension.

We performed further investigation of the effect of linear heat rate and the diffusion coefficient multiplier in an orthogonal array study, and looked at the strong main effects of both of these inputs with respect to the fraction FGR. We also calculated the variation factor which is a relative measure of the variation of the fraction FGR (over the variation in the diffusion coefficient multiplier) for a given LHR. The study confirmed that the uncertainties pertaining to the diffusion coefficient have a strong impact on code calculations. Also, our results provide an explanation to the known difficulty of properly predicting low FGR values as brought about – at least to some degree – by the uncertainties pertaining to the diffusion coefficient. Finally, we examined the calculated fission gas swelling at three locations. The variation factor for swelling was also quite high in some cases, pointing out the significant role of the diffusion coefficient uncertainties in fission gas swelling calculations.

These studies demonstrated the use of BISON, DAKOTA, and several statistical analysis methods which allowed us to investigate the sensitivity of the new model for fission gas behavior. These types of studies are useful both in code development as well as operational fuel rod studies.

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