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# Development of an Optimization Method for Fuel Design Parameters Using Sampling Techniques

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## Abstract

We propose an optimization method by using sampling techniques to get the optimal ranges of the fuel design parameters based on the fuel design criteria of the existing fuel rods. Using this technique, mechanical design parameters of dry processed fuel rods are optimized and compared with those of $UO_2$ fuel which was loaded to a pressurized water reactor. The modified FRAPCON-3 code system, which considers the new thermal models for the dry processed fuel is used. In the optimization process, important fuel fabrication parameters are selected and their sensitivities are estimated. The objective function for each design parameter is constructed using its safety margin. Then the resultant design values which minimize the objective function among many random samplings and Latin hypercube samplings were also used. It is expected that this method can be utilized to design new fuel concepts with enhanced performance and safety for future nuclear systems.

## 1. Introduction

Various nuclear systems of the future such as the generation IV reactor systems (Gen-IV) are being developed and international research programs will begin soon to develop new fuel concepts and revolutionary fuel cycles.[1] In Korea Atomic Energy Research Institute, dry process fuel was proposed and has been studied for the last 10 years.[2,3] Dry processed fuel cycle technology provides high proliferation resistance and better utilization of uranium resources. Also, this fuel cycle has the merit of minimization of the production of radiation wastes. The fabrication of a dry processed fuel pellet employs the OREOX (oxidation and reduction of oxide fuel) process followed by compaction and sintering. Some fission products except the volatiles in the spent fuel remain after fabrication. Thus, the performance of dry processed fuel is expected to be quite different form the existing $UO_2$ fuel. To evaluate the performance of dry processed fuel, the modification and expansion of the performance code system for $UO_2$ fuel is required. Those procedures will also be applied to new fuel performance for the revolutionary fuel cycle. The simulated fuel provides analogous behavior with the dry processed fuel which is fabricated from spent fuel.[3] Using the simulated fuel, the thermal and mechanical material properties were obtained to predict the in-reactor behavior of the dry processed fuel. The thermal performance of the dry processed fuel was evaluated under light water reactor condition with modification of the existing fuel performance code system.[4-6]

The fuel design parameters of the dry processed fuel should be optimized due to the different behavior of uranium oxide fuel in the reactor. Sensitivity analysis(SA) for fuel design parameters is performed in advance to know which parameter affects significantly the fuel performance. Sensitivity analysis is the study of how the variation in the output of a model (numerical or otherwise) can be apportioned, qualitatively or quantitatively, to different sources of variation, and of how the given model depends upon the information fed into it.[7] Among several methods of sensitivity analysis and uncertainty analysis, a sampling technique is considered to find the optimal design parameters of dry processed fuel. Random sampling and Latin hypercube sampling approaches are considered to find the optimal design parameters. The objective functions used are made from a combination of fuel design criteria, such as fuel centerline temperature and cladding temperature, strain, and cladding hydrogen pickup, etc. This approach of optimization for fuel fabrication parameters can be utilized as preliminary data for the design of dry processed fuel.

## 2. Fuel Rod Design Criteria for Pressurized Water Reactor

The fuel design criteria are slightly different for the nuclear system and the fuel fabrication companies, but all the design parameters are chosen within the bounds of a no radiation release accident. And normal operation and incident conditions (xenon oscillation, over power, etc) are considered to determine the fuel design parameters. The goal of fuel rod design is to maintain the robustness of the cladding which contains the nuclear fuel.[8]

Thermal power and burnup of fuel rod should be maximized to utilize nuclear fuel efficiently. To achieve those targets, it is necessary to understand the performance limit of the fuel and to evaluate quantitatively several characteristics of the fuel rod for irradiation. In the case of a pressurized water reactor (PWR), the American National Standard Institute (ANSI) conditions are used to design the fuel rod. ANSI condition I occurrences are operations that are expected frequently or regularly in the course of power operation, refueling, maintenance, or maneuvering of the plant. Condition II occurrences include incidents, any one of which can occur during a calendar year for a particular plant.[8,9]

Westinghouse 17X17 V5H fuel assembly, which is loaded in the Kori 3&4 plants, is used to evaluate the fuel design parameters.[9] Table I shows the design criteria for fuel rod design.

Table I. Design Criteria and Limits for Westinghouse 17×17 V5H Fuel

| Parameter | Condition I (normal operation) | Condition II (incidents of moderate frequency) |
|---|---|---|
| Fuel centerline temperature | < Melting temperature | |
| Rod internal pressure | < Enlarge the fuel-to-cladding gap | |
| Clad strain | < 1% from the unirradiated condition | < 1% from the pre-transient value |
| Clad stress | <0.2% offset yield stress | |
| Cladding temperature | < 672 K | < 700 K |
| Hydrogen pickup at cladding | < 600 ppm | |

## 3. Description of Code System

Among the thermal models of dry processed fuel for experiments, thermal conductivity and thermal expansion models are used for fuel performance calculation. Thermal conductivity model of dry processed fuel, which can be applied to 3000K, has been developed using the simulated dry processed fuel pellet. The basic model refers to $UO_2$ solid density from Harding and Martin. The suggested thermal conductivity model of dry process fuel for FRAPON-3 is given detail in reference 10. Fig. 1 shows the thermal conductivity for dry process fuel and $UO_2$ fuel.

The thermal expansion model of simulated dry processed fuel shows larger results than that of $UO_2$ fuel and the difference becomes larger as the temperature increases. The thermal expansion model of dry processed fuel is also given in reference 6. Fig. 2 shows the thermal expansion for dry processed fuel and $UO_2$ fuel.

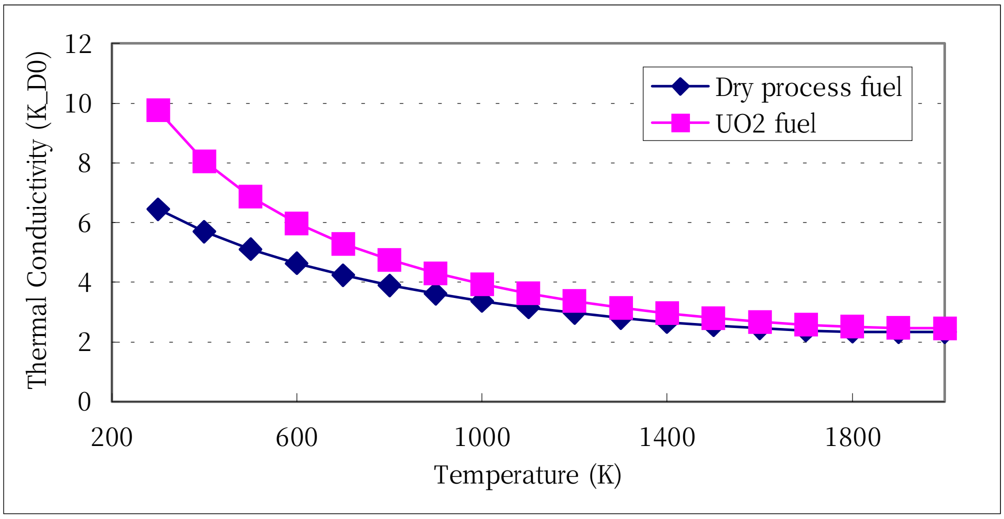


Figure 1. Thermal conductivity for dry process fuel and $UO_2$ fuel.

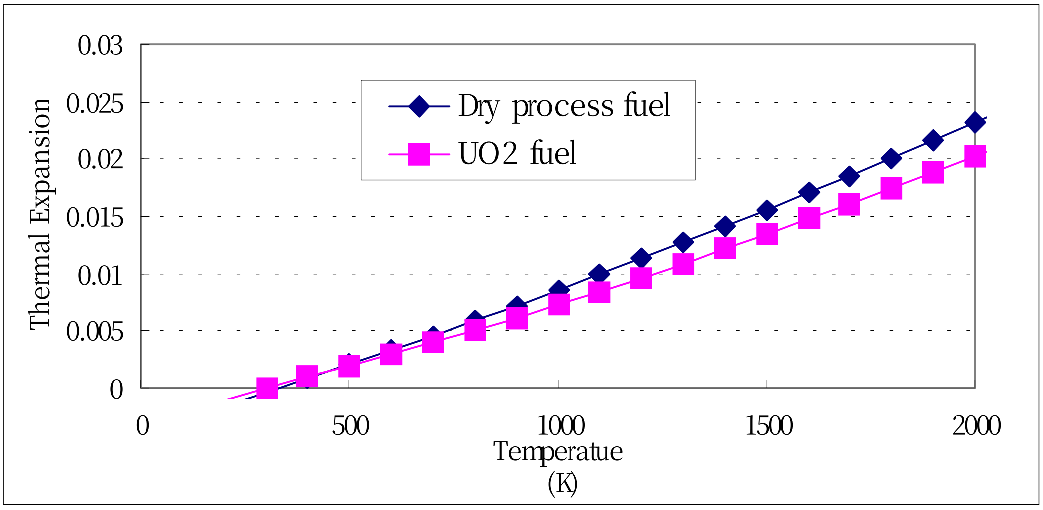


Figure 2. Thermal expansion for dry process fuel and $UO_2$ fuel.

## 4. Sensitivity Analysis for Design Parameters of Dry Process Fuel

### 4-1. Data Description

To derive the optimal dry process fuel design parameters, a sensitivity analysis of the fuel with FRAPCON-3 was performed. As expected, the behavior of dry processed fuel is quite different from the existing $UO_2$ fuel rod with irradiation. To obtain the temperature distribution using the new thermal model of dry processed fuel, 17X17 Westinghouse fuel rod resources are used in this work. For simplicity, burnup history is assumed to be constant from the beginning of life to the end of life and the reactor type is a light water reactor and the linear power rate is given as

17.85 kW/m. The enrichment of U-235 in the uranium is 3.912 wt%. The core data, fuel rod data, and fuel pellet data for this study are given in Table II, III, and IV, respectively.

The main design parameters which we want to investigate in detail are fuel theoretical density, pellet outer diameter, clad inner diameter, and the length of plenum. The variations of these parameters are given in Table V.

4-2. Results of Sensitivity Analysis

There are several definitions of sensitivity to find effects of fuel design parameters. The most popular sensitivity is a differential form such as

$$S_i = \frac{\partial y}{\partial x_i}, \tag{1}$$

where the quantity $S_i$ is the local sensitivity measuring the effect on output $y$ of perturbing input $x_i$ around a reference. In this case, $S_i$ is equal to one for all items.

Another sensitivity analysis provides for what happens to the output if all the inputs are allowed a finite variation. The derivative of Eq. (1) could be normalized by the mean of output and input. This kind of sensitivity is expressed as

$$S_i = \frac{\partial y}{\partial x_i}\frac{x_i}{y}, \tag{2}$$

and provides the information of the most influential factor.

Alternatively, the sensitivity index could measure the effect on output of perturbing input by a fixed fraction of input standard deviations, i.e.

$$S_i = \frac{\partial y}{\partial x_i}\frac{std(x_i)}{std(y)}. \tag{3}$$

In this paper, we used Eq. (2) as sensitivity to compare the effects of the exiting $UO_2$ fuel and dry processed fuel. Figs. 3, 4, and 5 show the sensitivities of pellet density for fuel centerline temperature, strain rate, and rod internal pressure with irradiation, respectively. In the case of fuel centerline temperature, both $UO_2$ and dry processed fuels have similar behaviors with negative sensitivities. Negative value of sensitivity means that the relation between the pellet density and centerline temperature is inverse proportionality. In general, when the density decreases, the porosity of the pellet increases and the thermal conductivity becomes lower, and thus the fuel centerline temperature increases.[11] And it is also considered for fabricating a pellet with suitable density without open porosity to avoid any moisture adsorption.[12] It is noted that the centerline temperature of the dry processed fuel is slightly higher than that of the $UO_2$ fuel due to the lower thermal conductivity of the dry processed fuel. The sensitivities of strain rate are all positive and both fuels have the same values until about 23,000 MWd/tHM. From 23,000 MWd/tHM, the sensitivity of the dry processed fuel becomes slightly larger due to the increased thermal expansion coefficient for a high temperature. The sensitivities of rod internal pressure provide similarly positive values for both fuels. If density increases, then pellet swelling does happen and thus the internal pressure naturally increases.

Figs. 6, 7, and 8 show the sensitivities for the cladding inner diameter. The fuel centerline temperature gives negative sensitivity around the beginning of the cycle (BOC) and becomes positive later. It could be interpreted that when the fuel temperature is low enough, the conduction depends on clad thickness but when the fuel temperature is high enough, the produced heat of a pellet is released sufficiently and thus is less dependent on the thickness of the cladding. Both $UO_2$ and dry process fuel show similar sensitivities of fuel centerline temperature for cladding inner diameter. The sensitivity of strain is significantly large comparing other parameters. Thus clad thickness is the most influential factor for strain as irradiation. $UO_2$ and dry process fuels provide similar sensitivities of strain and internal pressure, too.

Figs. 9, 10, and 11 show the sensitivities for a pellets outer diameter. Dry process fuel provides slightly smaller sensitivity for fuel centerline temperature and larger sensitivities for strain and rod internal pressure. This could be explained by the behavior of impurities in the dry processed fuel as the gap clearance changes. Dry processed fuel is expected to produce more fission gas and thus the conductivity decreases, which causes a higher fuel centerline temperature. Thus gap clearance should be adjusted to accommodate such phenomena of the dry processed fuel.

Figs. 12 and 13 show sensitivities of strain and rod internal pressure for plenum length, respectively. The sensitivity of fuel centerline temperature is omitted due to zero sensitivity, which means there is no relation between the fuel centerline temperature and plenum length. The sensitivities of strain and rod internal pressure are similar for $UO_2$ and dry processed fuels.

Table II. Core Data for Simulation

| Parameter | Value | Unit |
|---|---|---|
| Core Power | 2775 | MWT |
| Primary Coolant Pressure | 15.5 | MPa |
| Coolant Inlet Temperature | 564 | K |
| Coolant Mass Flow Rate | 3393 | $kg/s\text{-}m^2$ |
| Average Linear Power | 17.85 | kW/m |
| Maximum Accident Overpower | 118 | % |
| Heat Released Outside the Fuel Rod | 2.6 | % |

Table III. Nominal Fuel Rod Data

| Parameter | Value | Unit |
|---|---|---|
| Active Length | 3.66 | m |
| Rod Length | 3.87 | m |
| Plenum Length | 0.185 | m |
| Cladding Outside Diameter | 9.4996 | mm |
| Cladding Inside Diameter | 8.3566 | mm |
| Clad Thickness | 0.5715 | mm |
| Initial Gas Pressure | 1.90 | MPa |
| Upper End Plug | 11.4808 | mm |
| Low End Plug | 11.4808 | mm |

Table IV. Nominal Fuel Pellet Data

| Parameter | Value | Unit |
|---|---|---|
| True Density | 95.56 | % TD |
| Pellet Diameter | 8.1915 | mm |
| Pellet Length | 9.8298 | mm |
| Pellet Dish Radius | 12.827 | mm |
| Pellet Dish Length | 0.2413 | mm |
| Effective Chamfer Depth | 0.127 | mm |
| Effective Chamfer Width | 0.508 | mm |
| Fuel Enrichment | 3.912 | w/o |

Table V. Variational Data for Sensitivity Analysis

| Parameter | Nominal Value | Variational Value |
|---|---|---|
| True Density | 95.56 %TD | 94.56 %TD |
| Pellet Outer Diameter | 8.1915 mm | 8.2115 mm |
| Clad Inner Diameter | 8.3566 mm | 8.3366 mm |
| Plenum Length | 185 mm | 175 mm |

From the results of sensitivity analysis, the pellet’s outer diameter and clad inner diameter are the most influential factors on fuel centerline temperature and rod internal pressure. Clad strain rate is affected mostly by the clad inner diameter. Therefore, it is thought that gap clearance is one of the most important factors for fuel performance.

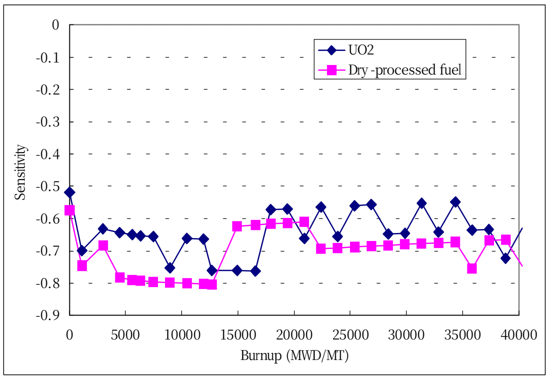


Fig.3. Sensitivity of fuel centerline temperature for fuel density.

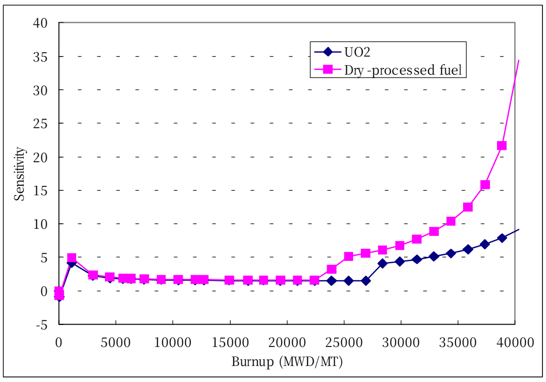


Fig.4. Sensitivity of strain for fuel density.

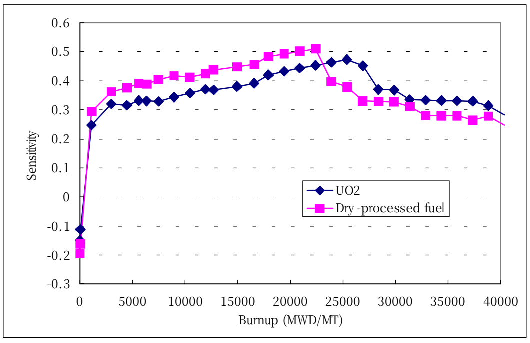


Fig. 5. Sensitivity of internal pressure for fuel density.

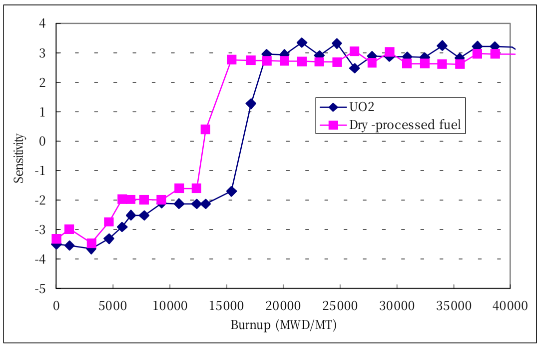


Fig. 6. Sensitivity of fuel centerline temperature for cladding inner diameter.

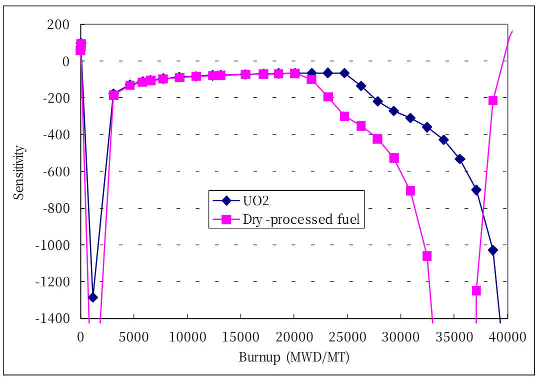


Fig. 7. Sensitivity of strain for cladding inner diameter.

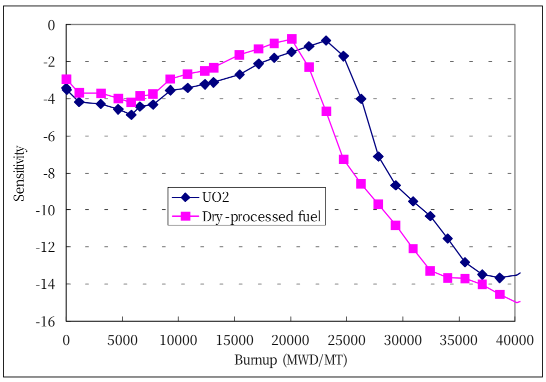


Fig. 8. Sensitivity of internal pressure for cladding inner diameter.

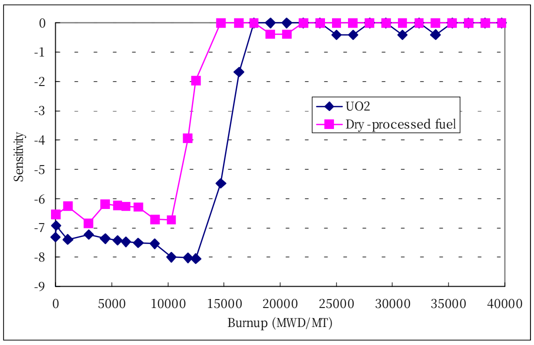


Fig. 9. Sensitivity of fuel centerline temperature for pellet outer diameter.

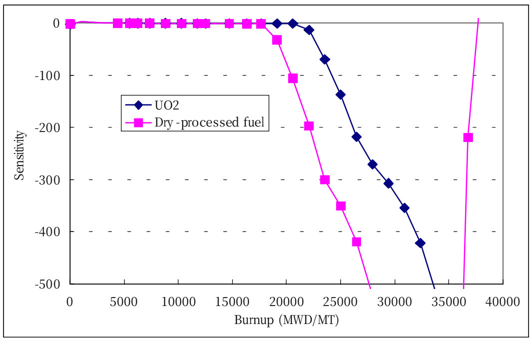


Fig. 10. Sensitivity of strain for pellet outer diameter.

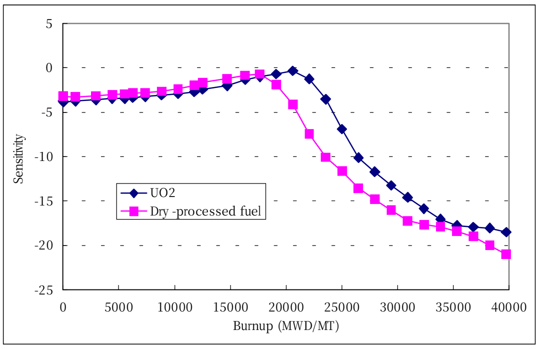


Fig. 11. Sensitivity of internal pressure for pellet outer diameter.

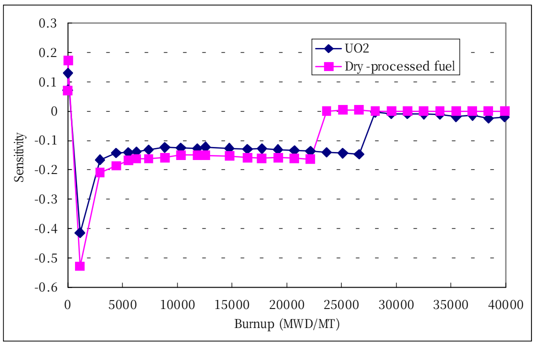


Fig. 12. Sensitivity of strain for plenum length

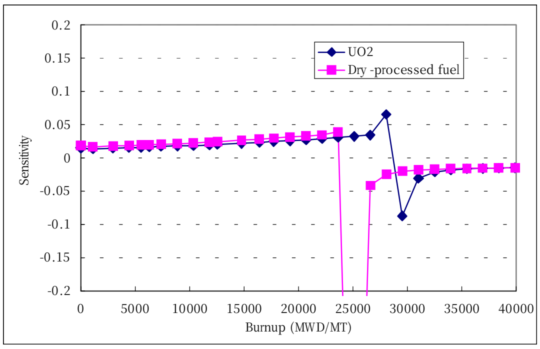


Figure 13. Sensitivity of internal pressure for plenum length.

## 5. Optimization Method Using Sampling Techniques

It is expected to exhibit quite different behavior when a dry processed fuel rod is loaded in the reactor instead of an $UO_2$ fuel rod. The design parameters of existing fuel rods are determined by several commercial code systems (PAD, COROSN, etc) and generic methods. Even a hand calculation is useful, for example the rod growth calculation. There are four significant fabrication parameters for the uncertainty in the rod's internal pressure. Clad inner diameter, pellet outer diameter, fuel density, and plenum length are influential factors. In this paper, the four parameters above are set to be optimized for the best fuel performance including rod internal pressure. The objective functions, which should be minimized, are defined from several major safety-related outputs, such as fuel centerline temperature, clad temperature, strain rate, and hydrogen pickup. The objective function used in this work is defined as

$$F(B) = \prod_{i=1}^{4} \frac{C_i}{C_i - D_i(B)}, \tag{4}$$

where $B$ is the burnup and the C's and D's are defined in Table VI.

Table VI. Design Safety Criteria for Objective Function

| Parameter (i) | Design Safety Criteria ($C_i$) | Code Outputs ($D_i$) |
|---|---|---|
| 1 | 3120 K | Fuel Centerline Temperature |
| 2 | 672 K | Clad Temperature |
| 3 | 1 % | Strain Rate |
| 4 | 600 ppm | Hydrogen Pickup |

The objective function may be defined differently and some weights could also be considered. To be simple, uniform weighting is used in this paper. The objective function should be minimized to optimize design parameters and if a certain parameter is very influential in design criteria, the objective functions will be large. Fig. 14 shows the configuration of the optimization method for fuel design parameters.

The sampling techniques are used to obtain input sets for the fuel performance code system. If N level is selected for four input parameters, $N^4$ input sets will be made, and it takes a tremendous computing time for enough levels. To reduce such a complexity, sampling techniques are useful. In this paper, we considered random sampling and Latin Hypercube sampling techniques.

### 5-1. Random Sampling

Sampling-based methods for sensitivity analysis involve the generation and exploration of mapping from uncertain analysis inputs to analysis results. It requires sampling procedures such as random sampling, importance sampling, and Latin-hypercube sampling. In the case of importance sampling, it is important to recognize that specifying variable distributions, number of strata, and strata probabilities does not uniquely define an importance sampling. Thus, only random sampling and Latin-hypercube sampling are considered here.

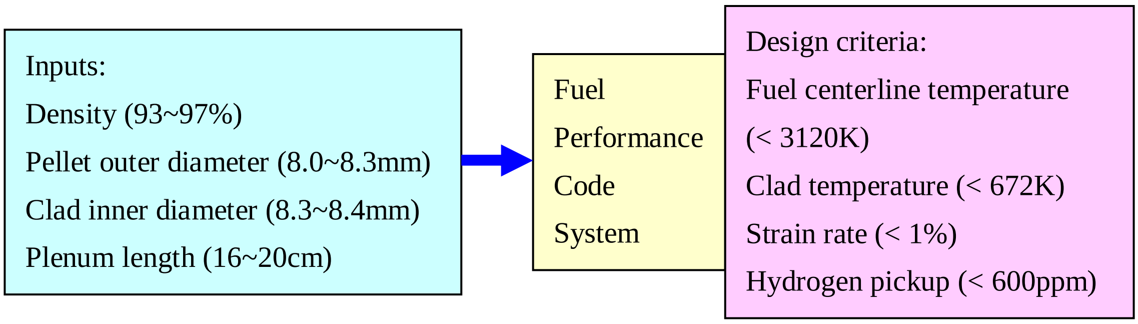


Figure 14. Configuration of optimization method for fuel design parameters.

In random sampling, sometimes called simple random sampling, the set of samples are sampled from a uniform distribution on normalized cumulative probability distribution ranges [0,1]. There are several fuel design parameters which are all independent and sampled randomly. It needs lots of simulation numbers to obtain sufficient confidence. If the input parameters are small this method is useful enough. Figs. 15 and 16 show the distributions of objective functions for $UO_2$ and dry processed fuels with irradiation, respectively. Each shows 10 simulation results for convenience. In the case of $UO_2$ fuel, simulation 1 exhibits strong robustness for long term burnup due to the increased objective function. Around 30,000 MWD/MT, simulations 6 and 8 show decreasing behavior thus they could be alternatives for optimized parameters. In simulation 9, some parameters are above the safety design criteria with irradiation. In the case of dry processed fuel, simulations 4 and 6 would be expected to be useful because they are decreasing around 30,000 MWD/MT. To obtain a more efficient sampling technique, Latin hypercube sampling is used.

5-2. Latin Hypercube Sampling

Random sampling is the preferred technique when sufficiently large samples are possible because it is easy to implement and provide unbiased estimates for means, variances, and distribution functions. The possible problems with random sampling derive from ‘sufficiently large’ sampling numbers. When random sampling is not computationally feasible for the estimation of extreme quantities, importance sampling is often employed. However, the use of importance sampling on nontrivial problems is not easy due to the difficulty of defining the necessary strata and also for calculating the probabilities of the theses strata. However, Latin hypercube is useful when large samples are not computationally practicable and the estimation of very high quantities is not required. Desirable features of Latin hypercube sampling include unbiased estimates for means and distribution functions and dense stratification across the range of each sampled variable. In some sense, Latin hypercube sampling can be viewed as a compromise importance sampling procedure when a priori knowledge of the relationships between the sampled and predicted variables is not available.[7]

The main difference between random sampling and Latin hypercube sampling is interval numbers when sampling form a cumulative distribution. There are no intervals for random sampling, but in Latin hypercube sampling, there are many intervals, as many as generation numbers. Thus, the distribution of intervals in Latin hypercube sampling is more uniformly distributed as shown in Fig. 17, which shows the distribution of samplings for two variables, plenum length and fuel density. Fig. 18 shows the results of simulations for dry processed fuel for 10 cases. As shown in Fig. 16 above, the behaviors of the objective functions are similar and among them, simulations 4 and 6 are preferable. Table VII shows the results of fuel design parameters from the simulations. These data are preliminary results and would be useful as basic data for realistic fuel rod design. From Table V, the density of the dry processed fuel rod could be lower than the existing $UO_2$ fuel rod.

From this simulation, only some fabrication parameters of fuel rods are chosen to be optimized and several safety design criteria are used. For more detail calculation, further available parameters should be considered and more realistic objective functions should also to be used.

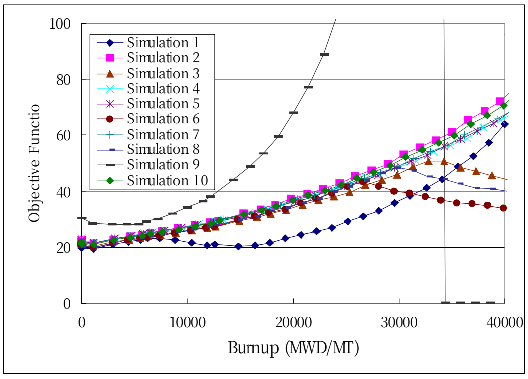


Fig. 15. Simulation of random sampling for $UO_2$ fuel rod.

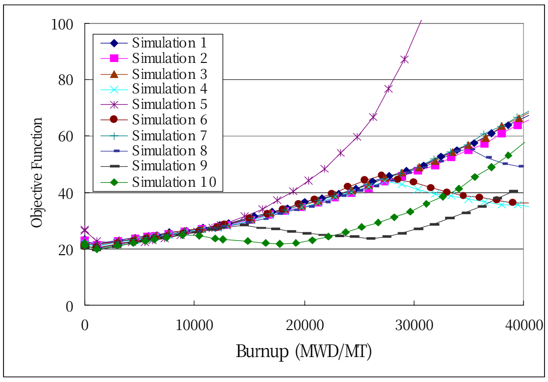


Fig. 16. Simulation of random sampling for dry process fuel rod.

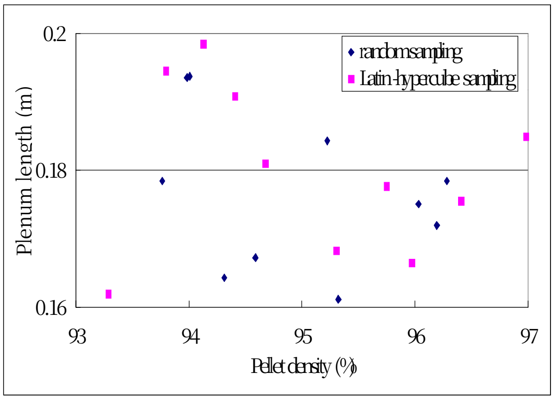


Fig. 17. Random sampling and Latin hypercube sampling.

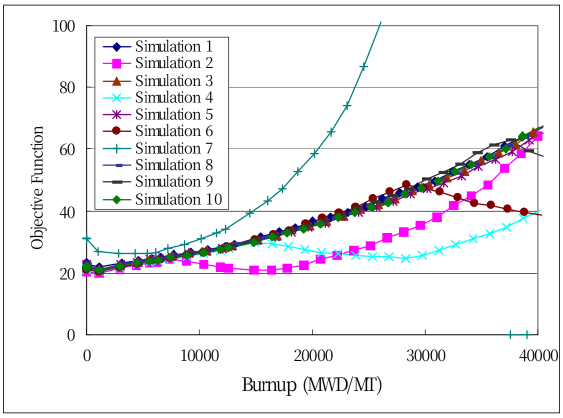


Fig.18. Simulation of Latin hypercube sampling for dry process fuel rod.

Table VII. Optimized Data for Dry Process Fuel Design

| Fabrication Parameter | Pellet Density (%) | Pellet Outer Diameter (mm) | Clad Inner Diameter (mm) | Plenum Length (cm) |
|---|---|---|---|---|
| Ref. (Westinghouse) | 95.56 | 8.1915 | 8.3566 | 18.5 |
| Random Sampling ($UO_2$) | 95.34 | 8.1440 | 8.3136 | 18.4 |
| Random Sampling (Dry process, sim4) | 93.86 | 8.1518 | 8.3216 | 18.1 |
| Random Sampling (Dry process, sim6) | 93.47 | 8.2160 | 8.3936 | 19.5 |
| Latin Hypercube (Dry process, sim4) | 94.83 | 8.1942 | 8.3366 | 19.6 |
| Latin Hypercube (Dry process, sim6) | 94.00 | 8.2176 | 8.4036 | 19.0 |

## 6. Conclusions

It is expected that dry processed fuel will exhibit quite different behavior compared with existing uranium oxide fuel and those characteristics should be considered for the fabrication of fuel rod design. As a fundamental step, a sensitivity analysis of several design parameters was performed to investigate the effect of each parameter on the performance of dry processed fuel. To optimize the significant fabrication parameters of the dry processed fuel rod, random sampling and Latin hypercube sampling techniques were used. The code system used was the modified FRAPCON-3 which contains thermal models of the dry processed fuel rod. From the simulation, we obtained the basic design data of the dry processed fuel rod which could be utilized for realistic fuel rod design. In the future, code systems could be updated considering thermal and mechanical models for dry processed fuel rods. To obtain more reliable design data from the optimization method, more design parameters and safety design criteria should be encompassed and realistic objective functions should be implemented. It is further expected that the optimization method of design parameters for the dry processed fuel rod will be directly applicable to various new fuel concepts for future nuclear systems.

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