OPTIMIZATION OF FAST FISSION GAS RELEASE MODEL PARAMETERS USING MACHINE LEARNING ACCELERATED EVOLUTIONARY ALGORITHMS

J.M. JOHNS, K.J. GEELHOOD

Pacific Northwest National Laboratory
902 Battelle Blvd. PO Box 999, Richland, WA 99352 USA

ABSTRACT

Fission gas release models used in FRAPCON and FAST are based on equations that describe the physical transport phenomena that control release from the fuel pellet to the rod void volume of fission gas produced during irradiation. Although these models are physically based, many of the parameters that control the release such as the impact of burnup on diffusion and bubble formation and saturation are critical to the accurate prediction of fission gas release, but cannot be measured in any quantitative way. To overcome this problem, these parameters have been empirically derived to provide a best fit to the available data that includes rod puncture data and electron probe microanalysis (EMPA) and X-ray fluorescence (XRF) data of radial location of residual gas within the pellet.

In general, a heuristic approach for deriving these parameters via practical implementation of expert analyses on just a few dependent variables has been shown to perform quite well in most situations. In this paper, we present an approach for applying machine learning to expedite model development. This approach is based on developing a deep artificial neural network which describes FRAPCON's fission gas release models, and optimizes parameters by a differential evaluation algorithm. This approach allows us to quickly and accurately tune physical models based on expert judgment, and works as a human-in-the-loop approach, to assist the modeler in identifying and addressing regions of high uncertainty in a multi-parameter space. Results of the updated fission gas release model will be shown for all the FAST assessment data.

1. Introduction

The fission gas release models in FAST [1] are based on the mechanisms known to control release from the fuel pellet to the rod void volume. Many of the specific parameters that control these processes are known to be impacted by a number of factors during irradiation such as temperature, burnup and neutron flux. It would be ideal if the specific parameters could be derived from a mechanistic understanding of the phenomena or from experiments designed to measure these parameters. However, there is currently no way to make a direct measurement of these parameters under typical conditions. Historically, what has been done to overcome this problem for the United States Nuclear Regulatory Commission (US-NRC) fuel codes is to establish a large database of fission gas behavior measurements that span a large range of operating conditions and then empirically derive the parameters that control the known fission gas release mechanisms.

This approach to calibrating the model parameters based on fits to these data sets has proved to be effective and the resulting fission gas release predictions have remained reasonable as more data have been added to the dataset.

The major drawback of this approach is that it can be quite time consuming and labor intensive to determine these model parameters. Additionally, currently there are two fission gas release

models in FAST that the user may select between and it is known that each provides good results in certain areas and less ideal results in other areas.

The goal of this current work is to use machine learning to automate the model parameter selection and to provide model parameters for a single fission gas release model that provides best-estimate predictions to fission gas release in all situations. Previous work that used neural networks to model fission gas release focused on using a neural network to predict fission gas release directly [2,3], while this work uses a neural network to predict specific parameters in the current semi-mechanistic model that had previously been empirically derived. After this fitting, the neural network is not used in future calculations, but rather the predicted parameters.

2.   Fission Gas Release Database

The data used to calibrate the fission gas release model parameters is described in greater detail in the FRAPCON integral assessment document [4]. This data set consists of four general sets of data;
- Rod puncture data from steady-state irradiation from rods irradiated to various burnup levels over a wide range of power levels and operating conditions
- Rod puncture data from slow and fast (12 hours to 5 seconds) power ramps to various power levels on rods and rod segments that had previously been irradiated to various burnup levels.
- Rod puncture data from steady-state irradiation from rods irriadiated to very high burnup (70-100 GWd/MTU) beyond the level that the fuel codes are typically qualified.
- Electron probe microanalysis (EPMA) and X-ray fluorescence (XRF) data from pellet cross sections that have been irradiated to various burnup levels at various powers. These data can be used to determine the quantity of residual fission gas that exists in the grains and on the grain boundaries.

Because the NRC fuel codes, FRAPCON and FAST are used to assess the predictions of vendor safety analysis codes it is critically important that they not significantly under predict fission gas release. Although the majority of fuel rods in a commercial light water reactor release very little fission gas (1-2%) it is those rods that release significantly more fission gas (5-20%) that are of regulatory concern as these are the rods that will challenge the safety limits related to rod internal pressure and fuel temperature. Therefore, the database used to assess the NRC fuel codes preferentially includes rods operated at higher power with higher release. Additionally, the uncertainty assessment that is performed on the codes is designed to assess the prediction of the rods with high release.

As the U.S. industry is moving toward operation to burnup beyond 62 GWd/MTU, it is important to assess the ability of the code to predict fission gas release at high burnup as a significant quantity (5-20%) of fission gas has been observed to be released from rods operating at moderate power levels that would not have released as much fission gas at lower burnups. With this in mind more puncture data have recently been added to the assessment database at higher burnup levels.

Finally, the addition of the EMPA and XRF data was included in order to provide initial gas distribution for a transient gas release model applied during reactivity initiated accidents where the time for diffusion is limited but the fuel temperature may increase rapidly causing a significant release in gas existing on the grain boundaries.

3.   Overview of FAST fission gas release models and assessment data

The two models used in FAST are both based on a two stage fission gas release model. In these models, the fuel rod is divided into axial nodes and radial rings. The gas produced in each ring is calculated based on the burnup in that area. The diffusion coefficient for fission

gas in UO_2 is calculated for each ring based on the temperature, burnup, and power level in each ring.

Diffusional release from the grains based on the average grain size is calculated for each ring based on the fission gas quantity in the grains, the diffusion coefficient for each ring, and the current time step size. This released gas is assigned to the grain boundaries.

Re-solution of some of the gas on the grain boundaries is determined based on the grain size and the diffusion coefficient for each ring. Finally, a grain boundary saturation concentration is determined for each ring based on temperature, grain size and gas pressure in the rod. When this saturation concentration is exceeded then gas on the grain boundaries from that ring is released to the void volume of the rod. No gas transport across various rings to the void volume is calculated and this is assumed to not be necessary as the fuel pellets are considerably cracked due to the large temperature gradient across the pellets.

The final source of fission gas release is an athermal release that is a function of pellet average burnup. This release is based on observations of fission gas release from rods with very low power levels where diffusional release does not predict any release.

The following section will provide a brief description of the two fission gas release models in FAST and the assessment of each model.

3.1. Modified Forsberg-Massih model

The modified Forsberg-Massih model uses the general solution method proposed by Forsberg and Massih [4] with modifications to the recommended model parameters to better fit the database of fission gas release. This was the original model in FRAPCON [6] and is the default model in both FAST and FRAPCON. The parameters have been fit to provide a best estimate prediction of high power steady-state data up to 70 GWd/MTU and power ramped data up to 62 GWd/MTU. This comparison is shown in Figure 1 and the standard deviation of the steady-state predictions is 2.6% absolute and the standard deviation of the power ramped predictions is 5.4% absolute.

When this model was compared to very high burnup (>70 GWd/MTU) data it did not provide a particularly good fit to the data. Additionally, it was never fit to predict the radial distribution of the gas remaining in the grains and does not predict this data well.
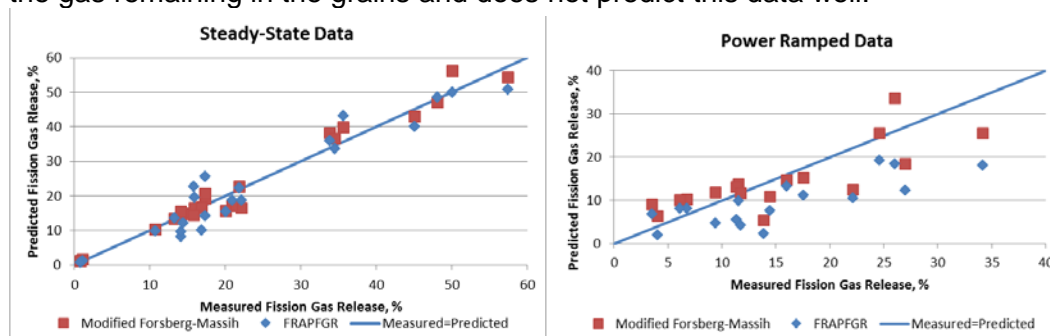

Figure 1: Steady-state and power ramped model to data predictions with both models

3.2. FRAPFGR model

In order to better predict the radial distribution of the gas in the grains and that on the grain boundaries and to better predict very high burnup data, the FRAPFGR model was developed. This model is based on the modified Forberg-Massih model, with several additional mechanisms included. These mechanisms include; a grain growth model and a high burnup

rim model. The high burnup rim model includes the restructuring of the grains to very small grains and in increase in the fuel porosity that is observed in the high burnup rim.

This model provides reasonable, but less ideal predictions of the steady-state and power ramped data with standard deviations of 4.3% and 8.1% for steady-state and power ramped data, respectively. These comparisons are shown in Figure 1 where it can also be seen that the FRAPFGR model underpredicts the high release ramp test data. It is also noted that the FRAPFGR model seems to underpredict the high release power-ramp data which is not desirable.

However, the FRAPFGR predicts very high burnup data considerably better than the modified Forsberg-Massih model as seen in Figure 2, and predicts the radial distribution of gas on in the grains well. Figure 3 shows an example of several of these predictions.
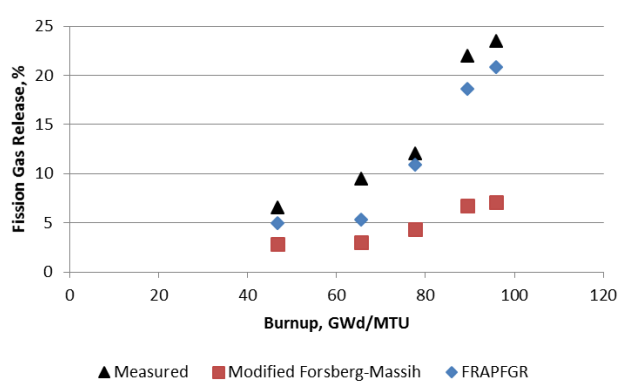

Figure 2: High burnup steady-state fission gas release data and predictions for both models
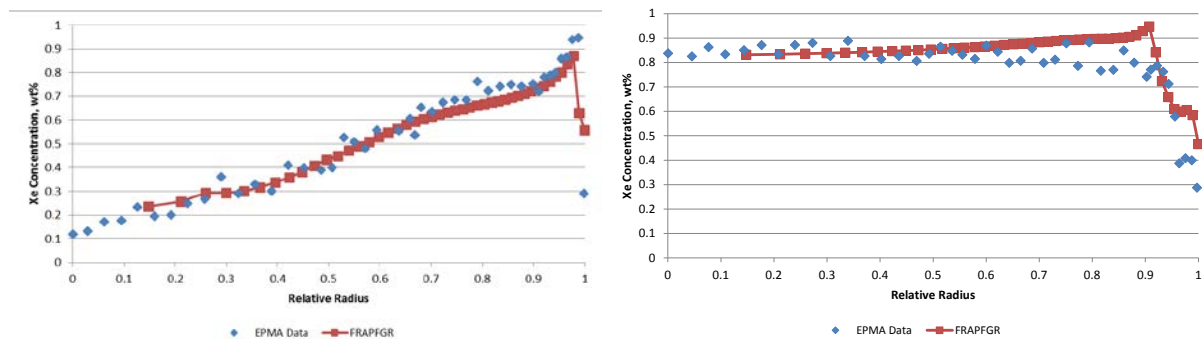

Figure 3: Example of predictions of the FRAPFGR model to radial distribution of gas within the grains

The goal of this work is to develop a single fission gas release model that provides good predictions of all of the available data.

4. Approach to model calibration using artificial neural networks

The fission gas release model, while developed with physical bases in mind, utilizes a number of parameters to perform empirical fitting to experimental data. The parameter fitting process is challenged by the nonlinearity in the relationships as well as uncertainties in experimental measurements. This nonlinearity in the parameter space necessitates a confluence of robust machine learning architectures capable of complex pattern recognition. The developed architecture is demonstrated in the flow diagram shown in Figure 4.
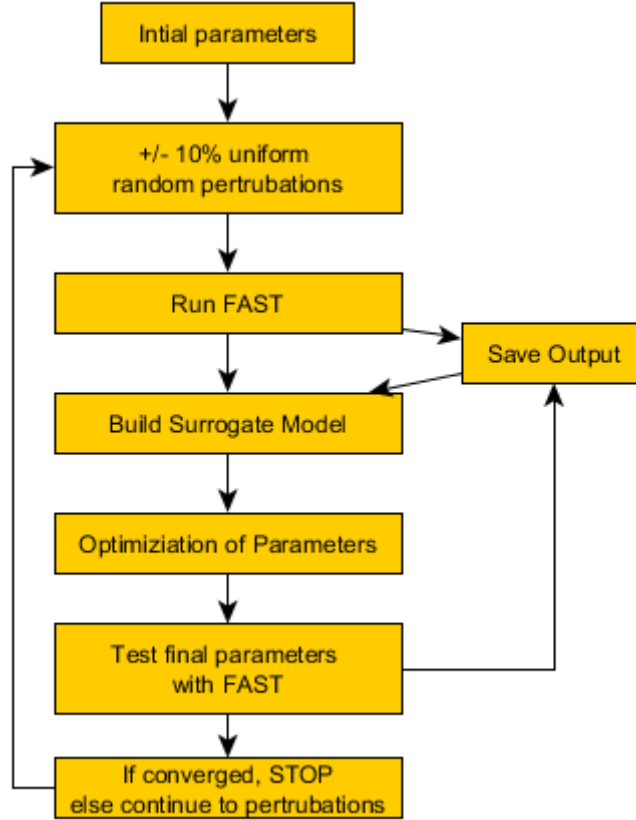
Figure 4: Flow diagram of parameter fitting process

The fitting process is enhanced by developing a framework of optimizing parameters such that a surrogate model can produce predictions of fission gas release accurately. The optimized parameters are tested within FAST, and the output generated then feeds into another iteration of the surrogate model. This optimization loop is continued until some convergence criteria is achieved. In this work, the loop is exited if the improvement no longer reduces the overall root-mean squared error of fission gas release predictions.

4.1. Problem Description

Let f be the response of FAST with given an input of z_i for experiment i with fission gas release model parameters, $\bar{x}$, then the fission gas release can be represented as:

$$y_i = f(\bar{x}, z_i) \qquad \text{Eq. 1}$$

where the error of the experimental measurements, Y_i, assuming no measurement uncertainty, and FAST is:

$$e_i = |Y_i - y_i| \qquad \text{Eq. 2}$$

Therefore, the objective function is a minimization on such that:

$$min_{\bar{x} \in R} = |Y_i - f(\bar{x}, z_i)| \qquad \text{Eq. 3}$$

4.2. Differential Evolution

The optimization technique utilized in this work is that of differential evolution (DE) [7], [8]. Differential evolution is a population-based, global optimization algorithm technique that is useful for multimodal problems where gradient-based methods fail. DE is a class of evolutionary algorithms, which utilize population selections to maintain diversity of the solution space in order to efficiently find globally minimized solutions.

Generally, the diversity is maintained, while simultaneously achieving improved fitness, by comparing candidate solutions with the current population of solutions and only survive (or continuing to the next iteration) if they possess higher fitness (or improve minimization) than the current population. The candidate solutions are generated according to the current population, utilizing many different rules. Those selected will be discussed here. The starting population is generated by a uniform random distribution over some starting interval.

All parameters are optimized with a bounding interval to allow for a stable optimization. This bounding interval, however, is allow to "walk" to the optimized solution, which is updated on each iteration. The progress is purposefully slowed with a relaxation factor. In particular, this is necessary due to the very large uncertainty in many parameters (like diffusion coefficient). Starting coefficient parameters intervals are set to be ±20% of their default value. The distributions are modified more slowly with a starting interval of ±8% of their default value due to the nature of the distribution searches. A Savitzky-Golay filter is used to smooth the response resulting from the random perturbation [6]. Despite the ±20% variation on the default value for coefficient, for example, this optimization scheme is able to explore the entire solution space as it gradually reaches a globally optimal solution.

Inevitably, evolutionary algorithms require many iterations to achieve convergence, and despite FAST running very quickly each realization, a surrogate model, $\hat{f}$, that can be run thousands of times a second is necessary to achieve convergence. The surrogate model is only an approximate representation of FAST:

$$\hat{f}(\bar{x}, z_i) \approx f(\bar{x}, z_i)$$
<div align="right">Eq. 4</div>

which is trained on a few hundred realization of FAST with random permutations of $\bar{x}$. A deep neural network was therefore explored as a potential option for modeling FAST as a surrogate model candidate.

4.3. Deep Neutral Network Architecture

Deep neural networks have become popular today for image classification of rather complex imagery due to their innate potential to learn highly nonlinear feature representations [7]–[9]. These were applied in this work to produce a low-order model between the fission gas release model parameter space and the error between the FAST predictions and measurements. Neural networks have been utilized to model fission gas release previously [10], [11], but this approach is distinctly different. The model is not built to represent data, but rather the performance of FAST as a function of the fission gas release model parameters.

Specifically, the surrogate model is trained to describe the error in FAST's predicted release to measured data, so Equation 4, is modified:

$$\hat{f}(\bar{x}, z_i) \approx |Y_i - f(\bar{x}, z_i)|$$
<div align="right">Eq. 5</div>

The surrogate model is only trained on a subset of the FAST solution (each FAST solution being one realization of a random set of parameters for all FGR validation case). The initial subset of the solutions is a total of 420 realizations. The neural network model used in this work is trained with 80% of the FAST realizations with the remaining 20% used to validate model performance. With each update from the global optimization, another 60 random parameters are used with the new optimal solution as a mean, increasing the number of realizations for training by 60 (see Figure 4).

Adagrad is used to optimize the network, with an initial learning rate of 0.004, and a linear decay rate for 250 epochs [12]. Rectified linear units were used for all activation functions, except for the output, which utilized linear functions. [13]

The final neural network architecture is displayed in Figure 5. The dense_X are fully-connected layers with X number of activation units, C1D_Y1,Y2,Y3 are 1-dimensional convolutions with Y1, Y2, and Y3, filters, kernel size, and strides. All convolution layers used valid padding. AvgPooling is average pooling with a pool size of 2, and dropout_Z is dropout with Z percentage of units randomly dropped. [14]
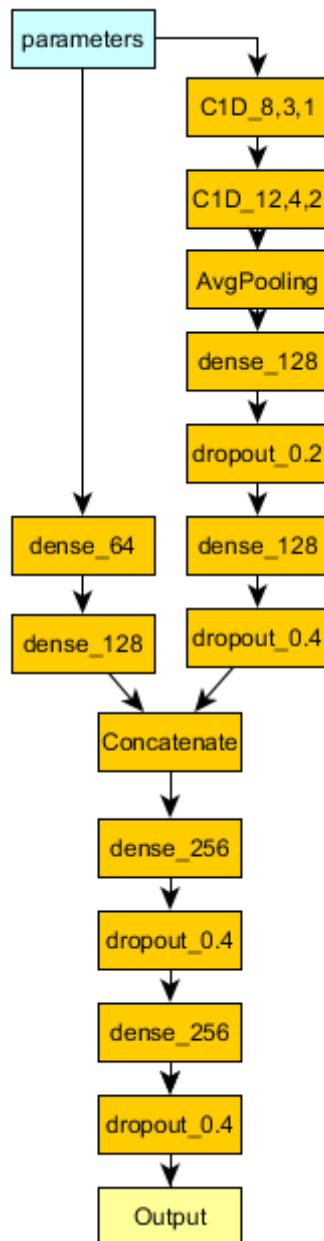
Figure 5: Artificial neural network architecture

4.4. Interface with FAST

A modified version of FAST was created to read coefficients for FRAPFGR model from a file to accomplish the optimization described above. In this way, the neural network could easily

modify these coefficients. The first part of this work was to identify the model parameters which had the smallest impact on fission gas release and radial distribution. This was performed by performing a sensitivity analysis explicitly using the surrogate model. With this, the model parameters that had minimal impact on fission gas release and radial distribution of gas were identified and eliminated. During this process, it was determined that the form of some models may not be appropriate to correctly model observed behavior and the final form of the models were included as a look-up table to give the neural network more flexibility. A new function is fit to these values after the values in the look-up table are optimized

5. Updated FRAPFGR model

The final results from the updated FRAPFGR model are shown in Figures 6, 7, and 8. The modified model provides reasonable predictions of the steady-state and power ramped data with standard deviations of 4.1% absolute FGR and 6.6% absolute FGR for steady-state and power ramped data, respectively. The model continues to provide good predictions of the very high burnup data as well as the radial distribution of gas on in the grains. As discussed in Section 2 the database preferentially includes rods with high release and the assessment uses an absolute standard deviation rather than a relative standard deviation as these are the rods that are most limiting from a safety perspective.
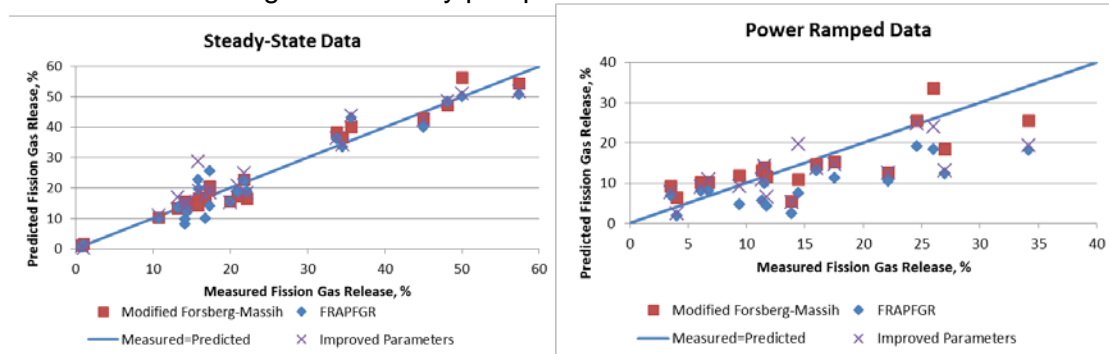

Figure 6: Steady-state and power ramped model to data predictions with updated FRAPFGR model
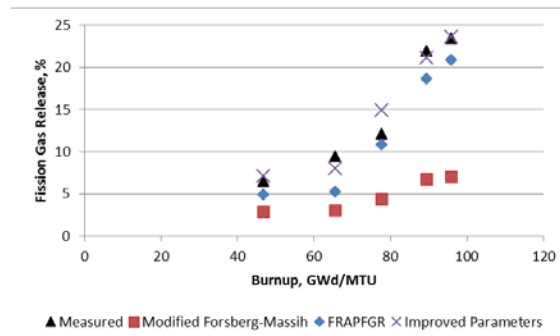

Figure 7: High burnup steady-state fission gas release data and predictions with updated FRAPFGR model
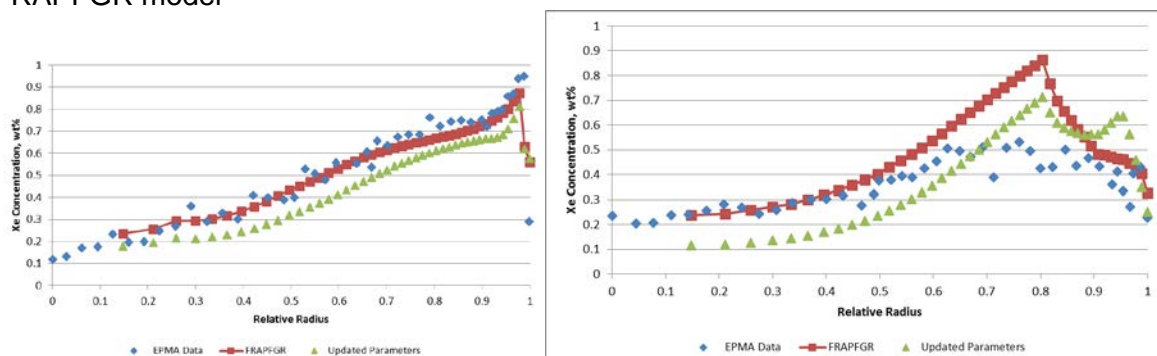

Figure 8: Example of predictions of the with updated FRAPFGR model to radial distribution of gas within the grains

6. Future use of artificial neural networks in fuel performance modeling

This application of an artificial neural network to inferring material behavior values could be used in other aspects of nuclear fuel performance modeling. Certainly, it could be applied to the fission gas release modeling of other fuel types such as mixed oxide (MOX) fuels or other advanced fuels. Additionally, it could be used to model fuel cracking and radial relocation in nuclear fuels, or pellet fragmentation and axial relocation during loss-of-coolant accident (LOCA).

This technique is available to any fuel performance phenomena where the general mechanisms that control the phenomena are known and a significant body of performance data are available, but the specific parameters that control these processes are not well known.

7. Conclusions

The fuel performance codes FRAPCON and FAST have contained two fission gas release models. The modified Forsberg-Massih model is the default model and applicable to steady state and power ramped rods up to 62-70 GWd/MTU. The alternate model, FRAPFGR, provides better predictions of very high burnup (>70 GWd/MTU) fission gas release and provides a good prediction of gas distribution radially within the fuel grains. This distribution is important in predicting fission gas release during severe accidents such as reactivity initiated accident and loss-of-coolant accident. The FRAPFGR also includes models for more of the phenomena known to change within the pellets during irradiation

A machine learning technique using an artificial neural network, with robust global optimization, such as differential evolution, was used to determine more ideal values for the empirical parameters within the FRAPFGR, such that it can provide estimates of fission gas release for steady state and power ramped rods that are as good as the modified Forsberg-Massih model while continuing to provide good predictions of very high burnup (>70 GWd/MTU) fission gas release gas distribution radially within the fuel grains.

This technique could be applied to other areas of fuel performance modeling and is available to any fuel performance phenomena where the general mechanisms that control the phenomena are known and a significant body of performance data are available, but the specific parameters that control these processes are not well known.

8. References

1. IE Porter, KJ Geelhood, WG Luscher. 2018. *FAST-1.0 Integral Assessment.* Publication Pending, U.S. Nuclear Regulatory Commission, Washington DC.
2. Yang-Hyun Koo, Jae-Yong Oh, Byung-Ho Lee, Young-Wook Tahk, Kun-Woo Song, 2010 "Artificial neural network modeling for fission gas release in LWR UO_2 fuel under RIA conditions", *Journal of Nuclear Materials*, Volume 405, Issue 1, Pages 33-43.
3. William S. Andrews, Brent J. Lewis, David S. Cox, 1999, "Artificial neural network models for volatile fission product release during severe accident conditions", *Journal of Nuclear Materials*, Volume 270, Issues 1–2, Pages 74-86
4. Geelhood, K.J. 2015, "FRAPCON-4.0 Integral Assessment, PNNL-19418, Vol. 2 Rev 2., Pacific Northwest National Laboratory, Richland, WA.
5. Forsberg K and AR Massih. 1985. "Diffusion Theory of Fission Gas Migration in Irradiated Nuclear Fuel UO_2." *Journal of Nuclear Materials* 135:140–148.
6. Geelhood KJ, WG Luscher, PA Raynaud, IE Porter. 2015. *FRAPCON-4.0: A Computer Code for the Calculation of Steady-State, Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup.* PNNL1-9418, Vol. 1 Rev. 2, Pacific Northwest National Laboratory, Richland, Washington.

7. E. Jones, T. Oliphant, and P. Peterson, SciPy: Open Source Scientific Tools for Python. 2015.

8. R. Storn and K. Price, "Differential Evolution – A Simple and Efficient Heuristic for global Optimization over Continuous Spaces," J. Glob. Optim., vol. 11, no. 4, pp. 341–359, Dec. 1997.

9. A. Savitzky and M. J. E. Golay, "Smoothing and Differentiation of Data by Simplified Least Squares Procedures.," *Analytical Chemistry*, vol. 36, no. 8, pp. 1627–1639, 1964.

10. A. Krizhevsky, I. Sutskever, and G. E. Hinton, "ImageNet Classification with Deep Convolutional Neural Networks," in Advances in Neural Information Processing Systems 25, F. Pereira, C. J. C. Burges, L. Bottou, and K. Q. Weinberger, Eds. Curran Associates, Inc., 2012, pp. 1097–1105.

11. Z. Wu, T. Yao, Y. Fu, and Y.-G. Jiang, "Deep Learning for Video Classification and Captioning," ArXiv160906782 Cs, Sep. 2016.

12. A. Canziani, A. Paszke, and E. Culurciello, "An Analysis of Deep Neural Network Models for Practical Applications," ArXiv160507678 Cs, May 2016.

13. W. S. Andrews, B. J. Lewis, and D. S. Cox, "Artificial neural network models for volatile fission product release during severe accident conditions," *Journal of Nuclear Materials*, vol. 270, no. 1–2, pp. 74–86, Apr. 1999.

14. Y.-H. Koo, J.-Y. Oh, B.-H. Lee, Y.-W. Tahk, and K.-W. Song, "Artificial neural network modeling for fission gas release in LWR UO2 fuel under RIA conditions," *Journal of Nuclear Materials*, vol. 405, no. 1, pp. 33–43, Oct. 2010.

15. J. Duchi, E. Hazan, and Y. Singer, "Adaptive Subgradient Methods for Online Learning and Stochastic Optimization," *J. Mach. Learn. Res.*, vol. 12, pp. 2121–2159, Jul. 2011.

16. K. He, X. Zhang, S. Ren, and J. Sun, "Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification," *arXiv:1502.01852 [cs]*, Feb. 2015.

17. N. Srivastava, G. Hinton, A. Krizhevsky, I. Sutskever, and R. Salakhutdinov, "Dropout: A Simple Way to Prevent Neural Networks from Overfitting," *J. Mach. Learn. Res.*, vol. 15, no. 1, pp. 1929–1958, Jan. 2014