INL/CON-23-73264-Revision-0

Preliminary Results for Uncertainty Quantification on Asymptotic Hydrogen Redistribution in a Prototypical Yttrium-Hydride Moderated Heat-Pipe-Cooled Microreactor

Changing the World's Energy Future

Quentin David Faure, Vincent M Laboure, Stefano Terlizzi

Idaho National Laboratory

INL/CON-23-73264-Revision-0

Preliminary Results for Uncertainty Quantification on Asymptotic Hydrogen Redistribution in a Prototypical Yttrium-Hydride Moderated Heat-Pipe-Cooled Microreactor

Quentin David Faure, Vincent M Laboure, Stefano Terlizzi

November 2023

Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

Prepared for the
U.S. Department of Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

Preliminary Results for Uncertainty Quantification on Asymptotic Hydrogen Redistribution in a Prototypical Yttrium-Hydride Moderated Heat-Pipe-Cooled Microreactor

Quentin Faure*, Vincent Labouré†, and Stefano Terlizzi†

*Department of Nuclear Engineering, North Carolina State University, 2500 Stinson Drive, Raleigh, NC 27695
†Reactor Physics Methods and Analysis Group, Idaho National Laboratory, 1955 N Fremont Ave, Idaho Falls, ID 83415
qdfaure@ncsu.edu vincent.laboure@inl.gov stefano.terlizzi@inl.gov

INTRODUCTION

Yttrium hydride (YH_x) is one of the most promising materials for moderating nuclear microreactors. This is due to its high hydrogen concentration at high operating conditions, large thermal conductivity, and chemical stability. However, when subject to thermal and concentration spatial gradients, the hydrogen tends to migrate within the yttrium matrix, potentially leading to power swings and reactivity changes. This paper aims to present preliminary results concerning the sensitivity of the thermal and hydrogen redistribution response for a prototypical heat-pipe-cooled yttrium-hydride moderated microreactor to thermal properties uncertainty and selected design characteristics. To the best knowledge of the authors, this is the first study examining the impact of uncertainties on microreactor hydrogen redistribution response. To achieve this goal, Bison [1] was used in conjunction with Dakota [2] to create a framework able to perform Uncertainty Quantification (UQ) for the Simplified Microreactor Benchmark Assessment (SiMBA) problem [3].

UQ METHODOLOGY

To obtain information on the impact of uncertain inputs on the temperature and H/Y ratio distribution, we rely on the two-step approach corresponding to the first two steps of the method discussed in Ref. [4]. The approach workflow is summarized in Fig. 1. After identification and characterization of input uncertainties, a global sensitivity analysis, using Morris screening, is performed to reduce the uncertain input space [5]. Such method relies on a small number of code evaluations, hence providing qualitative results while allowing to identify uncertain inputs with large impact on the output of interest.

The second step leverages the separation of epistemic and aleatoric uncertainties discussed in [6] (evidences of the importance of such input uncertainties treatment can be found in [4]). Epistemic uncertainties originate from a lack of knowledge (of the true value), while the aleatory uncertainties are from inherent stochastic processes. A range of values is used for the former, encompassing the true unknown value of the input, while evidence based statistical behavior is used for the latter. Therefore, an UQ based on a nested loop allows a consistent and accurate treatment of the input uncertainty's nature. The epistemic uncertainties are propagated on the outer loop using a full factorial grid (in our case, the extreme value of the epistemic uncertainty ranges), while the aleatoric uncertainties, using stochastic samplings (in our case, Latin hypercube sampling), are propagated in the inner loop. The use of the same stochastic samples at each epistemic grid points ensures meaningful comparison across all points. At each epistemic grid point, an aleatoric cumulative density function (CDF) is generated.

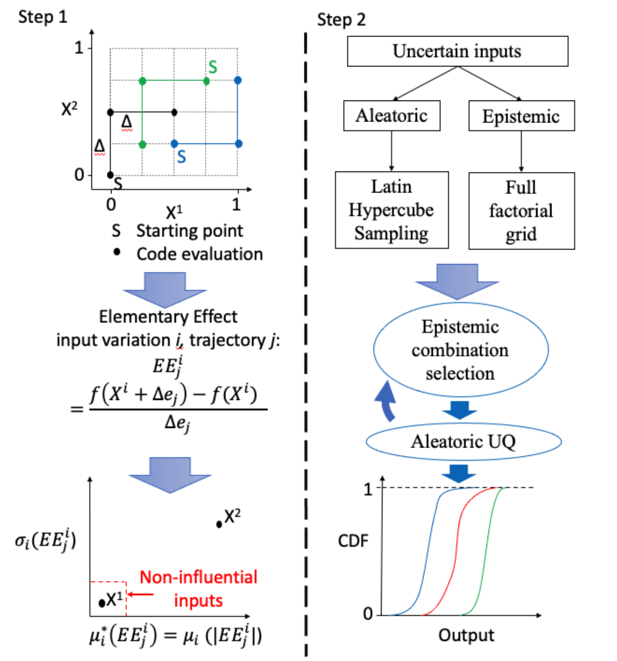


Fig. 1: Two-step approach flow diagram

COMPUTATIONAL PROBLEM

The SiMBA problem is a 2-MW heat-pipe cooled, YH-moderated microreactor. The reactor is composed of 18 hexagonal assemblies arranged into two rings. The tops and bottoms of these 160-cm-high assemblies are surrounded by 20-cm-high axial beryllium reflectors. Each assembly contains 96 fuel pins that are 1 cm in radius, 60 YH_x pins that are 0.975 cm in radius, and 61 1-cm-radius sodium HPs drilled into a graphite monolith. The HPs penetrate only into the top axial reflector, making the reactor axially asymmetric. The central shutdown rod slot is empty. The core is surrounded by 12 control drums, with boron carbide employed as the absorbing material. For a simplified mesh, the beryllium radial reflector is hexagonal. The geometries and material specifications of the SiMBA reactor assembly components are reported in Ref. [3].

The space-time evolution of the hydrogen stoichiometric ratio is computed in Bison [1] by solving the following system of coupled partial differential equations [3]:

$$\frac{\partial c}{\partial t} = \nabla \cdot D\left[\nabla c + \frac{Qc}{RT^2}\nabla T\right], \tag{1}$$

TABLE I: Uncertain inputs (and abbreviation) with their natures and statistical laws. The parameters distribution are the standard deviation for normal distributions and lower and upper bound for intervals

Input	Nature	Distribution	Distribution Parameters
Heat of transport (Q)	Epistemic	Interval	[1766, 15900] (J/mol)
Thermal conductivity fuel (tcf)	Aleatoric	Normal	10%
Thermal conductivity hydride (tch)	Aleatoric	Normal	see [7]
Thermal conductivity monolith (tcm)	Aleatoric	Normal	3.2%
Thermal conductivity Be reflector (tcb)	Aleatoric	Normal	5%
Effective heat transfer coefficient (h)	Epistemic	Interval	[366, 378] W/m^2K
Emissivity gap (eg)	Aleatoric	Normal	0.0333
Gap conductivity (gc)	Aleatoric	Normal	10%

$$\rho c_p \frac{\partial T}{\partial t} = \boldsymbol{\nabla} \cdot \lambda \boldsymbol{\nabla} T + P_d, \tag{2}$$

with D being the hydrogen diffusion coefficient in the metallic matrix, c the hydrogen/yttrium stoichiometric ratio, Q the heat of transport, R the universal gas constant, ρ the density, c_p the specific heat capacity, λ the thermal conductivity, and P_d the power density distribution (determined using the model in Ref. [3], approximately 2.3 MW/m^3). The heat transfer to the heat pipe is modeled using the following boundary condition:

$$\boldsymbol{J_q} \cdot \boldsymbol{n}^{hp} = h(T - T_{sink}), \tag{3}$$

where $\boldsymbol{J_q}$ is the heat flux at the boundary of the heat pipe, $\boldsymbol{n}^{hp}$ the unit normal vector to the boundary surface between heat pipes and gap, h the heat transfer coefficient, and T_{sink} the sink temperature of the heat pipe. In addition, the Bison gap heat transfer model is used to model the heat transfer between YH_x and cladding [1]. For the hydrogen redistribution, since we are interested in the asymptotic solution, we are assuming a zero net flux at the YH_x-gap interface, (*i.e.*, no hydrogen net desorption/adsorption). This can be translated mathematically into a zero Neumann boundary condition.

$$\boldsymbol{J_c} \cdot \boldsymbol{n}^{m} = 0. \tag{4}$$

In Eq.(4), $\boldsymbol{J_c}$ is the hydrogen current, while $\boldsymbol{n}^m$ is the normal unit vector associated to the moderator gap surface. In this work, Bison is used to solve Eqs.(1)-(3) using the Preconditioned Jacobian-free Newton-Krylov method. The Bison asymptotic solution was verified against analytical solution in past work [3].

RESULTS

Step 1: Morris screening

Table I reports the list of uncertain inputs used in this study and their corresponding statistical distributions. As shown in [3], material densities, heat capacities, and the diffusion coefficient play no role in the asymptotic solution, therefore, their uncertainties are not considered. Uncertainties on the geometry (manufacturing uncertainties) are generally extremely small based on [8], and are believed to have insignificant impact for this study due to solving for the temperature and hydrogen concentration only. In future work, these manufacturing uncertainties will be considered if the mechanical responses are implemented. The heat of transport, Q, is considered epistemic given that its value is not known. The range of variability was chosen large to ensure to bound its true value. The range for the effective heat transfer coefficient between monolith external surface and secondary fluid has been obtained from the Sockeye model used in Ref. [3]. The effective heat transfer coefficient is in general a function of the heat pipe geometry and material composition, therefore making the variation range reported in Table 1 likely underestimated. Future work will be devoted to perform UQ on the coupled heat conduction and fluid models, therefore explicitly accounting for the aleatoric uncertainties determining the variability range for h. Concerning the aleatoric uncertainties, they have been obtained from [8] [9] [7] [10]. The uncertainties on the hybrid thermal conductivity is varied between two standard deviations of the formula provided in [7], to encompass all the measurements from [11], especially for $YH_{1.72}$ to $YH_{1.86}$. The gap emissivity, gap conductance, and reflector thermal conductivity have fixed typical values in the BISON and their uncertainties correspond to potential variations of them. In addition to the epistemic and aleatoric uncertainties, the study is performed for two different heat sink temperatures to capture different operational scenarios: 800 K and 970 K.

The uncertainty quantification was performed on three outputs: maximum fuel temperature and maximum and minimum H/Y ratio in the moderator. Minimum fuel temperature, together with maximum and minimum temperatures for moderator, monolith, and reflector temperatures are also studied but not presented in this paper. In Fig. 2, the normalized results for the Morris screening of the maximum fuel temperature are shown for a sink temperature of 800 K. The normalization in Fig. 2 is performed using the maximum of the pseudo means (μ^*) and standard deviations (σ). The cutoff limit is generally empirical and was selected to be at 20% of the maximum to select only the most influential inputs [12]. It can be observed that only three uncertain inputs have influence and seem to have mainly a linear effect on the maximum fuel temperature, as expected. A global analysis of the results leads to the conclusion that only the gap emissivity is not influential for any output of interest. The gap conductivity is also deemed to be not influential when the sink temperature is 970 K, due to

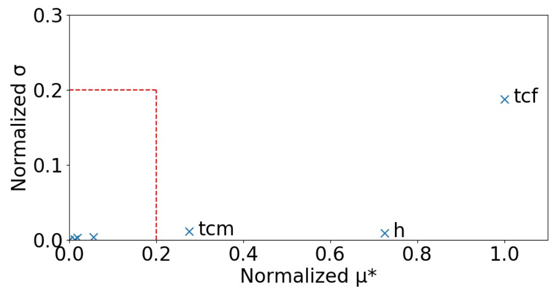


Fig. 2: Morris screening results for the maximum fuel temperature for a sink temperature of 800 K. The red dashed lines show the cutoff limit. For readability reasons, the legend is only shown for influential inputs.

being slightly below the cut off limit (for a sink temperature of 800 K, it is slightly above the cut off limit). The H/Y ratio is only influenced by the heat of transport. It is observed in all the results obtained, all the uncertain inputs have linear (standard deviation (σ) = 0, pseudo mean (μ^*)>0) or almost linear ($\sigma > 0$ but small, μ^*>0) impacts, for example as seen in Fig. 2 for conductivities and heat transfer coefficient [5].

Step 2: Nested UQ

The uncertainty quantification was performed using the nested approach explained in the UQ Methodology section. The heat transfer coefficient and heat of transport, the two epistemic uncertainties, are discretized to take only their respective extreme values. Based on Morris screening results, both uncertainties have linear effects on the output of interest, therefore any results obtained for values in between their bounds should lead to results in between to the ones obtained. Concerning the aleatoric uncertainties, the Latin hypercube sampling was used for each epistemic uncertain grid points with 120 samples and 150 samples for a heat pipe sink temperature of 800 K and 970 K, respectively. The number of samples are chosen to correspond to the number of uncertain inputs times 30. Figure 3 shows the maximum fuel temperature CDF for a heat pipe sink temperature of 800 K. The heat of transport, Q, having no impact on the temperature distribution (this statement would not hold true if the neutronics model were to be used, due to the feedback of the H/Y on the power), the results are presented only for variation of the heat transfer coefficient h. It can be observed that the maximum fuel temperature can vary by about five Kelvin total, which is relatively small. Concerning the heat pipe sink temperature of 970 K, the results are very similar but at higher temperature (average maximum temperature around 1050 K). The variations due to input uncertainties observed for the other material temperatures are below five Kelvin. Such small variations would not have major impact on the neutronics response of the reactor. However, a more complex and higher fidelity model than the one used for this study, might yield different results as more physics model would be implemented (i.e. fuel gas release, mechanical response, burnup, etc). Even though the variations ranges are similar in both sink temperature cases, the total ranges of temperature in the materials are different: for the same aleatoric and epistemic combinations, the fuel temperature varies by 56 K compared to 46 K for a sink temperature of 970 K and 800 K, respectively.

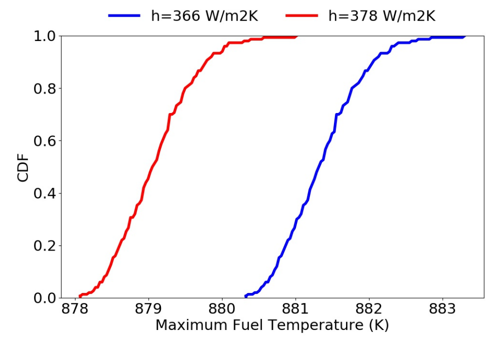
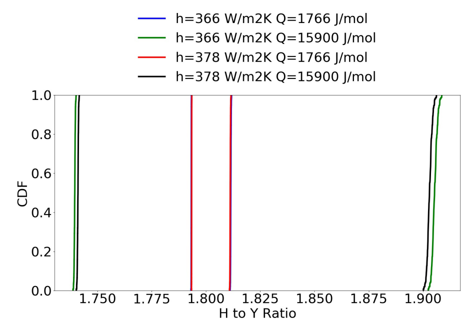
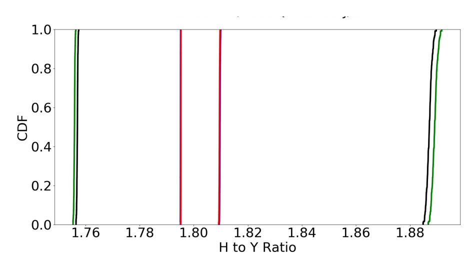


Fig. 3: Fuel maximum temperature CDF for a sink temperature of 800 K.

(a)



(b)



(c)

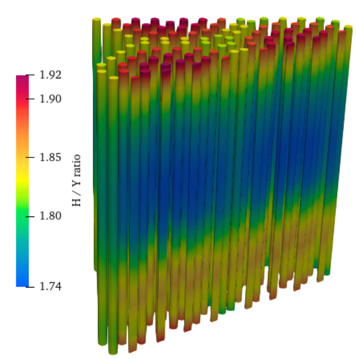


Fig. 4: H/Y ratio CDF for a sink temperature of (a) 800 K and (b) 970 K (h: heat transfer coefficient, Q: heat of transport). (c) axial view (z axis scale by 0.4) of the SiMBA problem for the a sink temperature of 800 K.

Fig. 4 presents the minimum and maximum H/Y ratio CDFs obtained for a sink temperature of 800 K and 970 K, as well as the H/Y ratio distribution corresponding to the maximum value of Q. As visible from Fig. 4.a, the H/Y ratio CDFs are almost vertical. This is because the heat of transport, an epistemic uncertainty, has the most influence on the H/Y ratio, therefore shadowing the impact of the aleatoric uncertainties. In addition, it is observed that the H/Y ratio can vary significantly (*i.e.*, between 1.74 to 1.92), even compared to the results reported in Ref. [3]. This large variation is explained by the large value chosen for the upper bound of the heat of transport. For $T_{sink} = 970K$, the variation of the H/Y ratio for different values of the heat of transport is smaller (maximum H/Y ratio between 1.81 to 1.89), which can be explained by a smaller the gradient of temperature. In fact, for $T_{sink} = 800K$, the moderator temperature variation is 45 K for an average temperature 851 K, while for $T_{sink} = 970\,K$, the moderator temperature variation and average temperature are 54 K and 1020 K, respectively. Therefore, in Eq.(1), the $\frac{1}{T^2}\nabla T$ term is higher for $T_{sink} = 800\,K$ compared to $T_{sink} = 970K$, leading to slightly larger variation of H/Y ratio for the lower heat pipe sink temperature case. Contrary to the temperatures, which seem to be varying over small ranges due to the uncertainties (aleatoric and epistemic), the variation of the H/Y ratio is expected to have a more significant impact on the neutronics response of the reactor. It is also noticeable from Fig. 4 that for $Q = 1766J/mol$ the curves computed at $h = 366W/m^2/K$ and $h = 378W/m^2/K$, respectively, overlap. This further confirm that the aleatoric uncertainties are negligible with respect to the epistemic uncertainties caused by the lack of knowledge of the heat of transport. The reason behind this is the proportionality of the Soret term in Eq. (1) to the heat of transport. Since the magnitude of Q is relatively small, the influence of the temperature gradient diminishes. Consequently, even when varying the aleatoric uncertainties, which impact temperatures within few degrees, their effect on the cumulative distribution functions (CDFs) presented in Fig. 4 remains negligible.

CONCLUSION AND FUTURE WORK

An uncertainty quantification study was performed on a Bison model of the SiMBA microreactor including heat transfer and hydrogen redistribution. The goal of this study was to quantify the effects of the physical uncertainties on the temperature and H/Y ratio distributions, which are feedback mechanisms for the neutronics modeling of the reactor. The analysis is performed for two different sink temperature and is limited to the asymptotic solution. In this model, uncertainties in thermal conductivities, heat transfer coefficients, and heat of transport are considered and categorized as epistemic or aleatoric. A nested approach for the uncertainty quantification, with epistemic uncertainties on the outer loop and aleatoric uncertainties in the inner loop is used. It is here shown that the uncertainties have minimal impacts on the temperature distribution (total variation around five K), but the heat of transport can strongly influence the H/Y distribution, which would have an impact of the neutronics response. It was noted that for the heat pipe sink temperature of 800 K, H/Y ratio spans on a slightly wider range compared to a sink temperature of 970 K. This is due to the gradient term in the hydrogen current equation that is larger in the first case. In conclusion, this investigation underscores the significance of acquiring a dependable experimental value for the heat of transport to precisely assess the influence of hydrogen redistribution in YH_x on neutronics. Furthermore, the study reveals a substantial effect of the sink temperature, along with a significant impact of the heat transfer coefficient, even within a small range of variation, likely influenced by the sink temperature. As a result, a more comprehensive examination of heat pipe uncertainties is warranted, which will be conducted in the future by coupling BISON and SOCKEYE.

ACKNOWLEDGMENT

This work is supported by the Idaho National Laboratory (INL) Laboratory Directed Research & Development (LDRD) Program under the U.S. Department of Energy (DOE) Idaho Operations Office Contract DE-AC07-05ID14517.

REFERENCES

1. R. L. WILLIAMSON et al., "Bison: A Flexible Code for Advanced Simulation of the Performance of Multiple Nuclear Fuel Forms," *Nuclear Technology*, **207** (2021).
2. B. ADAMS et al., "Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.15 User's Manual," Tech. Rep. SAND2020-12495, Sandia National Laboratory (2021).
3. S. TERLIZZI and V. LABOURÉ, "Asymptotic Hydrogen Redistribution Analysis in Yttrium-Hydride-Moderated Heat-Pipe-Cooled Microreactors Using DireWolf," *Annals of Nuclear Energy*, **186** (2023).
4. Q. FAURE et al., "Fuel Performance Uncertainty Quantification and Sensitivity Analysis in the Presence of Epistemic and Aleatoric Sources of Uncertainties," *Front. Energy Res.* (2023).
5. M. MORRIS, "Factorial Sampling Plans for Preliminary Computational Experiments," *Technometrics*, **33** (1991).
6. C. J. ROY and W. L. OBERKAMPF, "A Comprehensive Framework for Verification, Validation, and Uncertainty Quantification in Scientific Computing," *Nuclear Science and Engineering*, **200** (2011).
7. A. P. SHIVPRASAD et al., "Advanced Moderator Material Handbook," Tech. Rep. LA-UR- 20-27683, Los Alamos Scientific Laboratory (2020).
8. J. HOU et al., "Benchmark for Uncertainty Analysis in Modeling (UAM) for Design, Operation and Safety Analysis of LWRs," Tech. rep., Nucl. Energy Agency (2019).
9. S. T. ROSS et al., "Thermal Conductivity Correlation for Uranium Nitride Fuel Between 10 and 1923 K," *Journal of Nuclear Materials*, **3** (1988).
10. D. MCELIGOT et al., "Thermal Properties of G-348 Graphite," Tech. Rep. INL/EXT-16-38241, Idaho National Laboratory (2016).
11. M. ITO et al., "Thermal Properties of Yttrium Hydride," *Journal of Nuclear Materials*, **344** (2005).
12. P. TRENTIN et al., "Screening analysis and unconstrained optimization of a small-scale vertical axis wind turbine," *Energy*, **240** (2022).