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# Application of regression, variance, and density based global sensitivity methods to integrated VERA-CS and BISON simulations

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ABSTRACT

Uncertainty quantification (UQ) and sensitivity analyses (SA) are performed for coupled simulations between VERA-CS, a coupled pin resolved neutron transport and subchannel thermal hydraulics code, and the fuel performance code BISON. The interface between VERA-CS and BISON is performed in a multiphysics environment known as the LOCA Toolkit for U.S. light water reactors (LOTUS) currently under development at Idaho National Laboratory (INL). A focus is placed on using a variety of SA measures, including two regression based (Pearson and Spearman), one variance based (Sobol indices), and three moment independent measures (Delta moment independent measures with $L_1$, $L_2$, and $L_\infty$ norms). The problem under inspection is a single assembly depletion case for three fuel cycles. The figures of merit are the minimum departure from nucleate boiling ratio (MDNBR), maximum fuel centerline temperature (MFCT), and gap conductance at peak power (GCPP). SA results show MDNBR to be linear with consistent rankings throughout the fuel cycles. MFCT is linear, but with a change in rankings at the switch from open gap to closed gap models. GCPP is nonlinear at intermediate states that coincide with the onset of contact between fuel and cladding. These nonlinear states allow for the showcasing of higher order SA measures over first order methods.

## 1. Introduction

The current fleet of the U.S. nuclear power plants is expected to undergo a variety of technological developments including the use of accident tolerant fuel and higher burnup fuel to improve its economic performance. In order to help facilitate this shift, improved predictive methods are currently under development, in particular multiphysics environments.

The word multiphysics indicates a set of calculations involving multiple physical models. It is worth noting that it is rather arbitrary when a simulation enters the realm of multiphysics, as most engineering codes model multiple physical phenomena. For instance, legacy codes such as FRAPCON solve mechanical and thermal equilibrium equations as well as irradiative effects, oxidation, thermal hydraulics, and fission gas release. However, code documentation for FRAPCON (http://frapcon.labworks.org/, 2018) never refers to itself as a multiphysics code. This is partly due to the term being less common during the development of FRAPCON, but also due to the fact that all the phenomena receiving particular focus reside within the fuel performance discipline. The usage of multiphysics within this work implies the combining of interdisciplinary calculations which have commonly been treated separately in the past.

The definition of an environment in the computational context is amorphous as well noted by (Sloan et al., 2013). In this work, the word environment indicates a computational space in which users may utilize a variety of tools to generate, exchange, and process large amounts of data. Within this work, an environment is created that treats codes as modules which can readily and reliably be called upon in order to

*Abbreviations:* BEPU, best estimate plus uncertainty; CASL, consortium for advanced simulation of light water reactors; CIPS, crud induced power shift; CD-A, core design automation; CD-O, core design optimization; COBRA-TF, coolant-boiling in rod arrays-two fluids; FOM, figure of merit; GCPP, gap conductance at peak power; HPC, high performance computers; INL, Idaho national laboratory; LOCA, loss of coolant accident; LOTUS, LOCA toolkit for U.S. light water reactors; MCNP, Monte Carlo N-particle; MFCT, maximum fuel centerline temperature; MDNBR, minimum departure from nucleate boiling ratio; MPACT, Michigan parallel characteristics transport code; MOOSE, multiphysics object oriented simulation environment; NEAMS, nuclear energy advanced modeling and simulation; NEM, nodal expansion method; ORNL, Oak ridge national laboratory; PDF, probability distribution function; PWR, pressurized water reactor; RA, risk assessment; RIA, reactivity insertion accident; SA, sensitivity analysis; UQ, uncertainty quantification; VERA-CS, virtual environment for reactor analysis – core simulator

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perform large Monte Carlo samplings. This environment allows for the collaboration of multiple large scale projects for a more thorough modeling of designs to be employed in the nuclear industry.

Multiphysics studies have been implemented and studied extensively. In nuclear applications, work on multiphysics tends to focus on combining fuel performance, thermal hydraulics, neutronics, and/or isotopic depletion codes. Two multiphysics environments utilized by this work are the Virtual Environment for Reactor Analysis - Core Simulator (VERA- CS) (https://www.casl.gov/, 2018) developed by the Consortium for Advanced Simulation of Light Water Reactors (CASL) and the Multiphysics Object-Oriented Simulation Environment (MOOSE) developed at Idaho National Labs (INL). The version of VERA-CS used in this work performs tightly coupled calculations between the neutronics code MPACT, the thermal hydraulic code CTF, and the isotopic depletion code ORIGEN (see Section 2.1). MOOSE uses a modularized approach to allow for increased flexibility in code development. MOOSE employs fully-coupled, fully-implicit numerical methods to solve nonlinear equations within an adaptable, finite element framework (Gaston et al., 2009) (see section 2.2). This work uses the fuel performance code BISON, which is developed within MOOSE.

Notable instances of thermal hydraulics and neutronics coupling include the thermal hydraulics code Trace-PFI with a neutronics code based on the nodal expansion method (NEM) (Todorova and Ivanov, 2003) and a coupling of Monte Carlo based neutronics with subchannel thermal hydraulics (Sjenitzer et al., 2015). Examples of fuel performance and neutronics coupling include the fuel performance code TRANSURANUS and neutronics code DYN3D (Holt et al., 2015), and BISON with DeCART (Hales et al., 2015).

Couplings between fuel performance and thermal hydraulics include FRAPCON with TRACE-V5P3 (Porter et al., 2015) and BISON (https://bison.inl.gov/, 2018) with RELAP5-3D (Folsom et al., 2016). Furthermore a coupling between the transient fuel performance code FRAPTRAN, subchannel thermal hydraulics code COBRA-TF, and the neutronics code TORT-TD has been performed (Magedanz et al., 2015). A notable instance of a coupling between isotopic depletion and neutronics is the MCWO script (Chang, 2005) developed at INL which couples the isotopic depletion code ORIGEN2 with the Monte Carlo N-Particle transport code MCNP.

The Serpent Monte Carlo code (Leppänen et al., 2015) developed at the VTT technical center is also noteworthy for its widespread use in multiphysics studies, which include couplings of thermal hydraulics, computational fluid dynamics, isotopic depletion, fuel performance, and neutron and photon transport. Considerable work is also underway in the U.S. Department of Energy's program known as Nuclear Energy Advanced Modeling Simulation (NEAMS) to develop a workbench (Swiler et al., 2017) to handle the integration of neutronics, fuel performance, thermal hydraulics, and isotopic depletion codes. Finally the reactor and lattice physics code SCALE (Bowman, 2011) developed by Oak Ridge National Laboratory (ORNL) has been coupled with thermal hydraulic, computational fluid dynamics, and fuel performance codes. It is worth noting that the specified problem (i.e. reactivity insertion accident (RIA), loss of coolant accident (LOCA), quasi-steady state depletion) often varies among the aforementioned works.

An essential aspect in the development of multiphysics environments is the incorporation of uncertainty quantification (UQ) and sensitivity analysis (SA) methodologies. UQ and SA studies of multiphysics environments ensure that the results are not treated as absolutes, but rather as estimates with inherent uncertainty. In essence, UQ and SA studies assure that decision makers are privy to the best estimate plus uncertainty (BEPU) methodology which has become the de facto industry standard.

UQ and SA in reactor design and analysis had predominantly been used in the field of thermal hydraulics (Boyack et al., 1990; Marcum and Brigantic, 2015), but recently have been extended to fuel performance (Ikonen, 2016; Ikonen and Tulkki, 2014). UQ and SA have been performed on the fuel performance code BISON (Swiler et al., 2015; Pastore et al., 2015) using DAKOTA software, as well as with the RAVEN software developed at INL (Talbot et al., 2016). UQ and SA have also been extended to VERA-CS (Brown and Zhang, 2016; Brown et al., 2016). UQ has also been performed on VERA-CS via the Crud Induced Power Shift studies (CIPS) (Dinh, 2012). Notable UQ and SA have also been performed on SCALE (Williams and Rearden, 2008). UQ and SA on large multiphysics environments are still at their infancy and warrant further systematic studies.

In this work, a Monte Carlo based UQ and SA have been performed on an integration of CASL's VERA-CS code (https://www.casl.gov/, 2018) and INL's advanced fuel performance code BISON (https://bison.inl.gov/, 2018). The integration of VERA-CS and BISON and the subsequent UQ/SA studies are performed within the context of a multiphysics environment known as LOTUS which stands for LOCA Toolkit for the U.S. light water reactors.

For each instance in the Monte Carlo sampling, a VERA-CS output file was generated, from which the power histories and thermal hydraulic profiles for a pin of interest were inputted into BISON. The pin of interest in this case was defined as the pin with the highest linear heat rate at the end of the fuel life cycle. This selection criterion was chosen due to the fact that the fuel performance figures of merit (FOM) of this work always coincided with the highest power pin for all observed cases. While the maximum power pin changes location throughout the fuel cycle, a consistent pin location based solely on the maximum pin power at the end of three fuel cycles was used so as to maintain consistency. The outputs from VERA-CS and BISON were then used to obtain the FOM, from which all UQ and SA were performed.

The problem of interest presented in this work is a three cycle, single assembly, fuel depletion case. This case was selected based on its similarities with typical operational behavior of an assembly in a LWR. While ideally a full core would be simulated, a single assembly is more feasible for a Monte Carlo sampling given current computational limits. The quasi-steady depletion case will also eventually serve as a means of supplying initial conditions (particularly gap conductance) to LOCA cases which are to be the primary focus of future LOTUS studies as the name suggests.

The FOM for this case are the minimum departure from nucleate boiling ratio (MDNBR), maximum fuel centerline temperature (MFCT), and the gap conductance at peak power (GCPP). The GCPP results from BISON are of particular interest as past work with FRAPCON (Blakely et al., 2018), showed GCPP uncertainty to be highly nonlinear. This nonlinear behavior is likely attributable to abrupt shifts in certain empirical functions used within FRAPCON, as opposed to the more mechanistic models used within BISON (see Section 2.2).

All SA studies must decide upon which SA measure to employ and report among an ever expanding list of possible candidates. Each SA measure has advantages and disadvantages typically in the realms of required sample size and the ability to detect nonlinearities. The LOTUS environment provides a post processing toolkit for the calculation of a variety of SA measures for any set of recorded inputs and corresponding outputs. This work employs two regression based SA measures (Pearson and Spearman), one variance based (Sobol indices), and three moment independent measures (Delta Moment Independent (Borgonovo, 2007) with, $L_2$ and $L_\infty$ norm variations (Zhai et al., 2014).

Results show MDNBR to behave linearly and consistently among all SA measures and states throughout the fuel cycle. The most impactful inputs for MDNBR are the assembly power, inlet temperature, and outlet pressure. Lesser contributions also come from rated flow and clad outer diameter.

MFCT also behaves linearly with consistency among SA measures, but with significant shifts in SA measures from state to state. Initially, MFCT depends primarily on fuel thermal conductivity in addition to cladding inner radius and fuel radius due to their direct effect on gap conductance. Uncertainties of later states stem almost exclusively from fuel thermal conductivity, with lesser contributions from fuel density and assembly power due to their effect on burnup which in turn affects