M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

Multiphysics Simulation of Fission Gas Production and Release in Light Water Reactor Fuel with the MOOSE Application Redwing

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Abstract - *The MOOSE application Redwing was developed to couple the neutron transport and core simulator MPACT and the fuel performance program BISON in order to perform detailed, multiphysics simulations of LWR fuel pins. Redwing enables two-way data transfer of intrapin fields such as power density and temperature in order to improve the prediction of fission gas release and the overall accuracy of the simulation. An original algorithm was developed to enable transfer of fission gas data between MPACT and BISON, referred to as fission gas coupling. A fuel pin model based on the Watts Bar Nuclear 1 reactor was created, and several aspects of the model were studied: radial mesh and time step sensitivity, the effect of fission gas coupling on a single pin at constant power, and the effect of fission gas coupling on a fuel pin array that undergoes a shutdown. The results suggest that fission gas coupling has a significant effect on the solution for fuel pins at high power and high burnup.*

I. INTRODUCTION

Over the past few decades, there has been a trend in nuclear engineering to couple programs in order to perform multiphysics simulations. Along with this trend, there has been a drive to increase the detail of simulations in order to capture intra-fuel pin phenomena. Several of these phenomena are related to fission gas. Fission gas is a product of uranium and plutonium fission, which causes multiple issues in nuclear fuel rods: swelling, neutronic reactivity effects, and degradation of heat transfer between the fuel and cladding [1]. Fission gas is mobile in the fuel matrix, and over several years of burnup, a significant amount of the fission gas produced may be released into the fuel/cladding plenum, which is known as fission gas release. Fission gas release is a complex phenomemon; besides steady release of fission gas at constant power, it is possible to trigger additional fission gas release via sudden changes in the fuel rod power (e.g. during a reactor shutdown); this is known as transient fission gas release.

There are several software packages that were used to perform this study. BISON [2] is a fuel performance application of the Multiphysics Object-Oriented Simulation Environment (MOOSE), which is under development at Idaho National Laboratory (INL). BISON is able to solve the nonlinearly coupled solid mechanics and heat transfer equations that model a fuel rod as it is depleted in a nuclear reactor. BISON relies on the finite element framework of MOOSE to discretize the problem geometry. BISON has a module called Sifgrs [3] which includes physics-based models for the important aspects of fission gas behavior.

MPACT [4, 5] is a 3D neutron transport and reactor core simulator based on the method of characteristics (MOC). The development of MPACT began at the University of Michigan (UM) and now is under the joint development at Oak Ridge National Laboratory (ORNL) and at UM as part of the DOE CASL Simulation Hub. MPACT is able to model the inter-pin effects of local assembly elements and is able to calculate intra-pin quantities such as the 3D multigroup neutron flux, fission rate density, and power density fields. MPACT uses the 2D/1D method to solve the neutron transport equation. This method solves the 2D, axially-integrated neutron transport equation with MOC for multiple axial slices of the domain; these planar solutions are coupled via a 1D axial solver. MPACT also solves the Bateman equations in order to track fuel composition changes with burnup; this is referred to as fuel depletion.

Redwing is an experimental MOOSE application which enables coupling between MPACT and BISON for fuel depletion simulations, usually 3-5 years in duration. Redwing was initially developed in collaboration between INL and UM, and is currently under development at UM. Redwing combines MPACT and BISON into a single executable, and all coupling is done in-memory. Rather than simulating an entire reactor core, Redwing simulations are limited to several fuel pins with detailed meshes. Two-way transfer of intra-pin data fields are used to couple MPACT and BISON. Redwing has not yet been validated, but it has been demonstrated with several simulations of PWR fuel [6]. There are separate, ongoing validation efforts for both BISON and MPACT [7, 8].

The objective of this work is to investigate and to develop a full-physics, consistent fission gas coupling method using MPACT and BISON. Both MPACT and BISON calculate a distribution of fission gas in the fuel; with fission gas coupling, it is possible to obtain a solution with consistent fission gas distributions on the two meshes, so that the coupled simulations have more accurate predictions of fission gas release and are more accurate overall.

II. COUPLING METHOD

Redwing maps and transfers the intra-pin fields of fission rate density, power density, fast neutron flux, and fission gas concentration from the MPACT mesh to the BISON mesh. For a two-way coupling, Redwing maps and transfers the intra-pin fields of temperature and fission gas concentration back to the MPACT mesh. Data are transferred based on the original coordinates of the BISON mesh, to avoid the need to remesh in MPACT when fuel and cladding deformation occurs on the BISON mesh. Loose coupling is employed with MPACT and BISON taking matching time steps; a time step sensitivity study (see Section IV.) demonstrates that this method yields reasonable solutions.

Algorithm 1 (in Appendix) shows how Redwing advances the solution from time i to time $i+1$; it does not specifically refer to MPACT and BISON, but it was created with MPACT and BISON in mind. For example, 19 Xe and Kr nuclides are considered, which is based on MPACT's depletion library. MPACT depletion simulations may be run with ORIGEN from the SCALE package, but for this study MPACT's internal depletion solver with MPACT's depletion library was used. Also, steps 12-15, which constitute the undeformed fuel/cladding plenum treatment, are necessary because the MPACT mesh is fixed. This special treatment was motivated by the desire to reduce errors in the MPACT solution without enabling mesh deformation in MPACT; the treatment essentially redistributes fission gas in the undeformed MPACT plenum according to how much gap closure has occured.

The nuclear engineering community has implemented two-way code coupling in various ways. In the case of Redwing, all the underlying code is compiled along with the Redwing code into the one executable. First, MPACT is compiled as a collection of static libraries, and then the code for MOOSE, MOOSE modules, BISON, and Redwing are all compiled as a single program and linked against the MPACT static libraries. In order to achieve communication between Redwing and MPACT, the subpackage `Coupler_Redwing` was created in MPACT; this subpackage calculates and holds data for transfer to BISON, and provides interfaces for Redwing to transfer data from BISON to MPACT. Redwing can run multi-pin problems using MOOSE's `MultiApps` system; for these cases, each app is almost an independent program, but they are all linked by the underlying MOOSE system. Figure 9 in the appendix gives a visualization of the breakdown of Redwing during runtime for a multi-pin simulation.

Redwing can be run on multiple processes via spatial decomposition of the computational meshes; with this approach, each process runs the same program. There is an `MPI_WORLD_COMM` communicator created by Redwing that is passed into the MPACT initialization subroutine, so that everything is on the same communicator. In the future, multiple communicators may be used for more efficient computation (e.g. creating a new MPI communicator for each BISON fuel pin mesh).

III. PROBLEM DESCRIPTION

The fuel pin model used in this study is based upon the VERA Core Physics Benchmark Progression Problems from CASL [9]; the focus of these problems is simulating the Watts Bar Nuclear 1 (WBN1) reactor. WBN1 uses fuel rods typical of a PWR; see the cited CASL report for the fuel rod specifications. The mechanical contact, thermal contact, and materials models are almost all the same as those used in the VERA model of WBN1. A recent improvement in the Redwing models is the use of the finite deformation formulation for solid mechanics; this results in a more accurate solution.

MPACT and BISON retain their own meshes when coupled via Redwing. MPACT is always run with a 3D mesh, while BISON is run with a 2D RZ mesh to reduce the computational expense of the simulations. Although the radial dimension of the fuel is small, radial meshing is very important for both neutron transport and fuel performance due to the large variation in power density. For the base case, the fuel was divided into four annular elements between the centerline and surface to create the MPACT mesh, which is one more than MPACT's default number of radial fuel elements; the base BISON mesh was required to have 11 finite elements along the radial direction, so that each MPACT mesh element contained at least one BISON mesh element centroid. The cladding was split into 1 and 3 radial elements in the MPACT and BISON meshes, respectively. The coolant had 11 radial mesh elements in the MPACT mesh, and the coolant was not included in the BISON mesh. Based on the CASL Progression Problem, MPACT had 62 mesh elements along the axial direction in the fuel; BISON had 500.

For all results presented in this paper, Redwing took five time steps during a three hour startup ramp; after this point, the time step was increased to a larger, fixed value. For the base case, this larger value is 20 days, which is common for MPACT depletion problems. The MPACT solver uses a boron search for each time step until the moderator boron concentration fell below zero; then the MPACT solver switched to the power method to compute the eigenvalue k_{eff}. The MPACT solver used MPACT's 47 energy group neutron cross section library, version 4.1. The internal depletion solver in MPACT was used to update the intra-pin nuclide density fields; this solver used MPACT's depletion library found in the `MPACT_Extras` repository.

The coupled simulations performed in this study yielded a large amount of data which can be considered part of the solution: there are many field quantities which vary with position in the fuel rod and time, as well as quantities which come from spatial integrals or averages. Most of the analysis is focused on spatial integrals or averages, in order to more easily draw conclusions. Henceforth, these will be referred to as quantities of interest (QOIs). Because fission gas coupling is the focus of this study, several QOIs are fission gas-related:

- Net fission gas production (i.e. amount of fission gas produced minus amount that is transmutated to other nuclides in fuel)
- Fission gas released to the plenum (an integral over time of the fission gas release rate)
- Fission gas inventory in plenum (accounts for gain due to release and loss due to transmutation in the plenum.)
- Average gap width

Other QOIs examined in this work are related to nuclear reactor operation and safety. These quantities are outlined in the Nuclear Regulatory Commission's Standard Review Plan document [10]. These quantities include:

- The neutron transport eigenvalue, k_{eff}

- The maximum fuel temperature, which is one of the main indicators of fuel integrity
- The average fuel temperature
- The maximum strain on the cladding. According to the NRC [10], the uniform strain must be limited to 1%, not including creep and irradiation growth. This limit is in place to preserve cladding integrity. The cladding strain reported in Section IV. is not separated by its physical causes; however, the 1% limit is still a useful reference value.

IV. RESULTS AND ANALYSIS

In the interest of reproducibility, the version numbers or Git commit hashes are given in Table I to show the exact versions of the codes used to obtain results. All codes required by Redwing are under development. These results were obtained with a version of MPACT that was branched off of master on 2016 Oct. 30 in order to simplify the development process.

1. Meshing and Time Step Sensitivity

The radial densities of the MPACT and BISON meshes were varied to determine the sensitivity of QOIs. This sensitivity study was performed on a model of a single WBN1 fuel pin with reflective boundary conditions set on the sides and vacuum boundary conditions on the top and bottom for neutron transport. Table II shows the results of this study. The MPACT mesh was comprised of 4, 8, 16, or 32 mesh elements between the fuel centerline and the fuel surface. Due to restraints of the data transfer method, these MPACT radial meshings corresponded to BISON meshings of 11, 12, 27, and 57 elements, respectively. For reference, most BISON PWR assessment problems are run with only 11 finite elements along the radial direction.

At the end of the simulation, t = 1280 days, the differences in the QOIs between the 16/27 and 32/57 MPACT/BISON radial mesh cases were only a few percent, suggesting that the 16/27 radial mesh case is sufficiently refined. The difference in both fission gas released and plenum fission gas inventory between the 16/27 and 32/57 cases is only -3%, which is encouraging; these are the two most important QOIs in this study. Figure 1 shows the evolution of the percent fission gas released; the small bump in this quantity at t = 60 days is likely transient fission gas release triggered by a change in temperature; it corresponds to a small amount of fission gas release.

There are large relative differences in the gap width at t = 1280 days, which are not reported in Table II. The gap is practically closed at this time, as shown in Figure 2, so small absolute differences in gap width correspond to large relative differences. All radial meshing cases agree well on the predicted gap width. At about t = 1280 days, all cases predict the beginning of clad liftoff; it starts slightly earlier in the 4/11 radial meshing case, which can be seen at the bottom-right corner of Figure 2. t = 1280 days corresponds to a burnup of 59 MWD/kgHM, which is physically too early for clad lift-off to occur; various modeling inaccuracies contributed to this early prediction, including the omission of spacer grids.

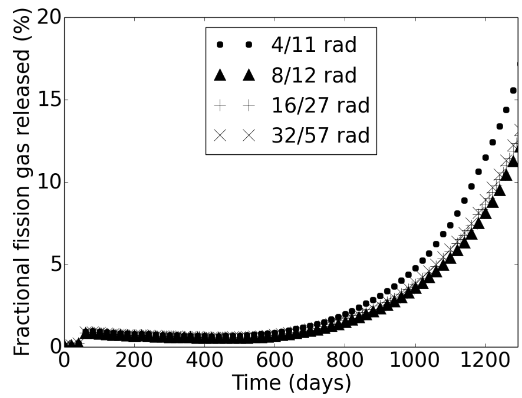

Fig. 1: This is the percent of fission gas released (i.e. fission gas released divided by net fission gas generated) for four different radial meshing cases. The cases are reported as the number of MPACT radial mesh elements / the number of BISON radial mesh elements.

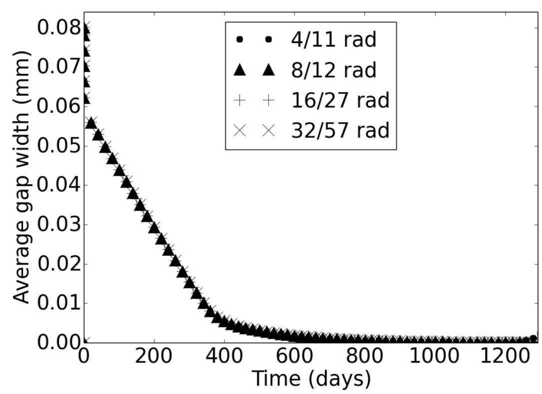

Fig. 2: The gap width averaged over the length of the fuel for four different radial meshings; 0.084 mm is the initial gap width.

Table III shows the results of a time step sensitivity study. By default, Redwing makes the MPACT and BISON solvers take the same time step, but sometimes BISON is subcycled in order to achieve convergence. The time step sizes reported are those set by Redwing; however, for all cases BISON had to be subcycled on at least a few Redwing time steps.

As expected, most QOIs show improvement in accuracy with the reduction in the time step size, such as the percent fission gas released shown in Figure 3. Two exceptions to the expected behavior are the maximum cladding hoop strain and net fission gas produced. The relative error in maximum cladding hoop strain hovers around 0.8%, which is acceptably small. The net fission gas produced is significantly higher

Code	Git SHA-1 hash or version number	Commit date
Redwing	`d0bfc3a361`	2017 Feb. 2
MPACT (branch)	`0fb938d4ab`	2016 Dec. 2
MPACT (master)	`10bc0f11ce`	2016 Oct. 30
BISON	`34ebe05f3d`	2017 Jan. 11
MOOSE	`fe73a4caad`	2017 Jan. 17
libMesh	`5129e936af`	2016 Dec. 7
PETSc	`3.6.3`	2015 Jun. 9

TABLE I: Code versions used for this chapter

Output quantity	Most refined: 32/57 rad	4/11 rad	8/12 rad	16/27 rad
Avg. fuel temperature	1150 K	3.16%	-0.92%	-0.40%
Max. fuel temperature	1646 K	3.64%	-0.94%	-0.37%
Max. cladding hoop strain	0.00907	10.15%	-2.28%	-1.04%
Fractional FG released	12.25%	27.23%	-7.90%	-3.35%
Net FG produced	0.134 mol	-0.01%	-0.01%	-0.00%
Plenum FG inventory	0.0164 mol	27.23%	-7.87%	-3.37%
FG released to plenum	0.0165 mol	27.22%	-7.90%	-3.36%
k_{eff}	0.813315	43 pcm	2 pcm	6 pcm

TABLE II: Relative differences in quantities of interest and absolute difference in k_{eff} compared to the most refined case for the MPACT/BISON radial mesh sensitivity study

for the dt = 5 days case. This behavior is likely the result of time-integration error due to using loose fission gas coupling along with MPACT's internal fuel depletion solver, resulting in the overproduction of Xe and Kr gas. Although unexpected, this increase in error is small, with only a 1.5% difference between the dt = 5 days and the dt = 2.5 days cases.

Although the dt = 20 days case has significant relative error in the fission gas released and the plenum fission gas inventory at 7% to 8%, this time step size was chosen to run further simulations. The reduction in error with decreasing time step was only a few percent (these quantities were seemingly less than first-order accurate), so using a time step size smaller than 20 days is not worth the increase in computing time. The time-integration error in net fission gas produced in the fuel (mentioned above) results in the slow error reduction in the QOIs fission gas released and plenum fission gas inventory.

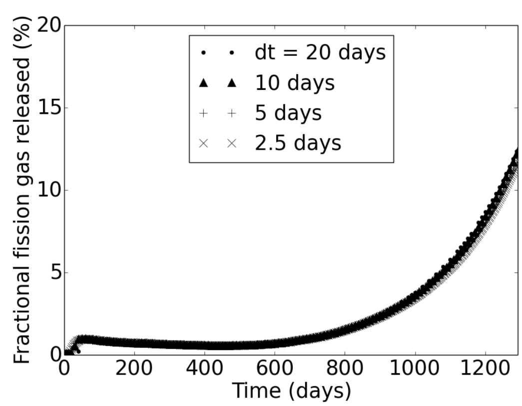

Fig. 3: Percent of fission gas released (i.e. fission gas released divided by net fission gas generated) for four different time step cases

2. Effect of Fission Gas Coupling on a Single Fuel Pin Model

The primary way to evaluate fission gas coupling is to compare two cases which are identical except for the activation of fission gas coupling. Table IV shows the effects caused by enabling fission gas coupling; for decoupled fission gas, the fission gas quantities reported are those calculated by the BISON solver. Note that more data are shown at variable time intervals; this is due to subcycling the BISON solver.

Coupling the fission gas fields caused a significant increase of about 9% in fission gas-related QOIs, like plenum fission gas inventory and fission gas released; as expected, the coupling also effected the overall solution to the coupled problem, as evident in the change in maximum fuel temperature and maximum cladding hoop strain. Figure 4 shows the increase in percent fission gas release caused by fission gas coupling. These changes occured mainly because fission gas coupling results in higher net production of fission gas in the fuel; the higher fission gas production rate is partially due to the increase in the plutonium fission rate with burnup, which has a higher yield than uranium of fission gas nuclides and precursors; BISON's Sifgrs model does not take this effect

Output quantity	Most refined: dt =2.5 days	20 days	10 days	5 days
Avg. fuel temperature	1140 K	0.53%	0.46%	0.34%
Max. fuel temperature	1633 K	0.40%	0.42%	0.29%
Max. cladding hoop strain	0.00891	0.71%	0.83%	0.79%
Fractional FG released	11.11%	6.56%	5.54%	3.13%
Net FG produced	0.134 mol	0.60%	0.61%	1.47%
Plenum FG inventory	0.0147 mol	7.62%	6.73%	5.00%
FG released to plenum	0.0149 mol	7.20%	6.18%	4.65%
k_{eff}	0.813385	0 pcm	3 pcm	-2 pcm

TABLE III: Relative differences in quantities of interest and absolute difference in k_{eff} compared to the most refined case for the time step sensitivity study

into account when the fission gas fields are decoupled. The higher fission gas concentration in the fuel results in higher release.

Table IV shows the same value for plenum inventory and fission gas released for the decoupled case because there is no distinction between these quantities with decoupled fission gas fields. Part of the fission gas coupling algorithm (see the appendix) is to account for loss of fission gas in the plenum due to transmutation, which necessitates the transfer of the fission gas released to the neutron transport solver. The loss of fission gas in the plenum is evident from the fact that the relative difference in the plenum inventory, 9.08%, is slightly smaller than the relative difference in gas released, 9.46%; as noted, these differences are relative to the same value. This suggests that the effect of transmutation in the plenum is small for this particular model.

Output quantity	FG decoupled	FG coupled
Avg. fuel temperature	1135 K	0.93%
Max. fuel temperature	1618 K	1.35%
Max. cladding hoop strain	0.00861	4.19%
Fractional FG released	11.02%	7.40%
Net FG produced	0.132 mol	1.92%
Plenum FG inventory	0.0145 mol	9.08%
FG released to plenum	0.0145 mol	9.46%
k_{eff}	0.812760	62 pcm

TABLE IV: Relative differences between quantities of interest and absolute difference in k_{eff} caused by coupling the fission gas fields

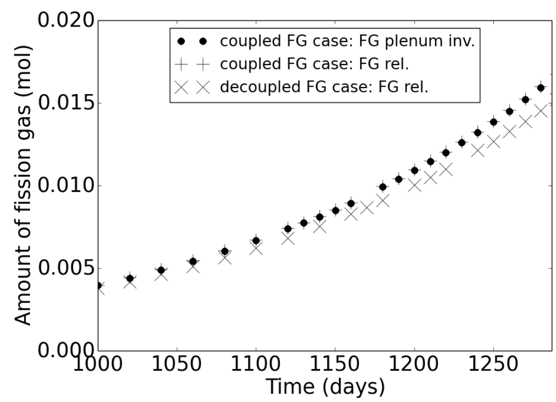

Fig. 4: This is a comparison between coupled and decoupled fission gas cases of fission gas released near the end of life for the single fuel pin model. Also included is the fission gas plenum inventory for the coupled fission gas case. For the decoupled fission gas case, there is no distinction between the fission gas released and the plenum inventory.

3. Effect of Coupling Fission Gas on a Fuel Pin Array with a Reactor Shutdown

In order to investigate the effects of fission gas coupling on the neutronic interaction between fuel pins, a small fuel pin array model with reflective side boundary conditions was created. Like the single pin model, the neutron transport boundary conditions on the top and bottom of the domain were vacuum. Figure 5 depicts the pin array model. A guide tube filled with water was placed in the upper left corner to create a tilt in the pin power distribution. All other pins contained fuel. The model could be thought of as a quarter of a 5x5 pin array with a central guide tube. A shutdown of 3.5 days occured at t = 900 days, which is roughly the length of two fuel cycles. The end of this simulation was at t = 1160 days.

Eight fuel pins were explicitly modeled with MPACT and BISON meshes; five fuel pins had unique solutions due to symmetry. Like with the single pin simulations, the MPACT mesh was 3D, while the BISON fuel pin meshes were 2D, extending in the axial and radial directions. Fields transferred from MPACT to BISON were first averaged over the azimuthal angle. Based on the single pin mesh sensitivity studies, the 16/27 radial meshing was used for each fuel pin and the maximum time step was set to dt = 20 days.

The power of the pin array was set such that the array's average pin power was 110% of the average pin power of WBN1 during normal operation; a 120% power simulation was attempted, but this resulted in convergence issues with the BISON solver. The hottest fuel pins were the two directly adjacent to the empty guide tube, and the coldest pin was the one farthest from the guide tube. At the end of the simulation,

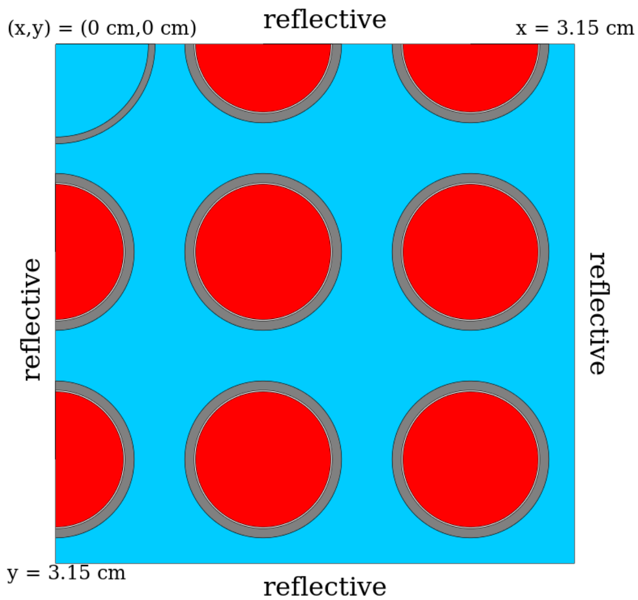

Fig. 5: A cutaway view of the midplane of the pin array model. Red is fuel, blue is moderator, gray is Zircaloy, and white is helium in the fuel/cladding gap. Reflective boundary conditions for neutron transport were set on all four sides of the domain.

the hottest and coldest fuel pins were at 112% and 109% of the average pin power for WBN1, respectively. For WBN1 The difference in the hottest pin's power caused by coupling the fission gas fields was only 1 W, an insignificant amount.

Table V shows the differences in the hottest pin's QOIs caused by enabling fission gas coupling. Small yet significant differences can be seen in the fission gas QOIs; however, these differences are much smaller than those seen in the QOIs for the single pin problem (see Table IV). This suggests that the importance of fission gas coupling is mainly dependent on the pin power, rather than other factors such as intrapin neutronic interactions or rapid power level changes.

Output quantity	FG decoupled	FG coupled
Avg. fuel temperature	1020 K	0.05%
Max. fuel temperature	1424 K	0.19%
Max. cladding hoop strain	0.00001	-0.48%
Fractional FG released	2.98%	0.86%
Net FG produced	0.113 mol	1.72%
Plenum FG inventory	0.00336 mol	1.93%
FG released to plenum	0.00336 mol	2.60%
Pin Power	75302 W	0.00%
k_{eff}	0.838002	11 pcm

TABLE V: Relative differences in quantities of interest and absolute difference in k_{eff} for the hottest pin in the array caused by fission gas coupling

Figure 6 shows k_{eff} over the simulation period. k_{eff} started at 1.00000 and remained fixed until the boron search yieled zero, and then the MPACT solver switched to solving the eigenvalue problem, so k_{eff} began to decrease. There was a brief spike in k_{eff} caused by the decrease in fuel and moderator temperature during the shutdown. This plot demonstrates that enabling fission gas coupling has a negligible effect on k_{eff} for this model.

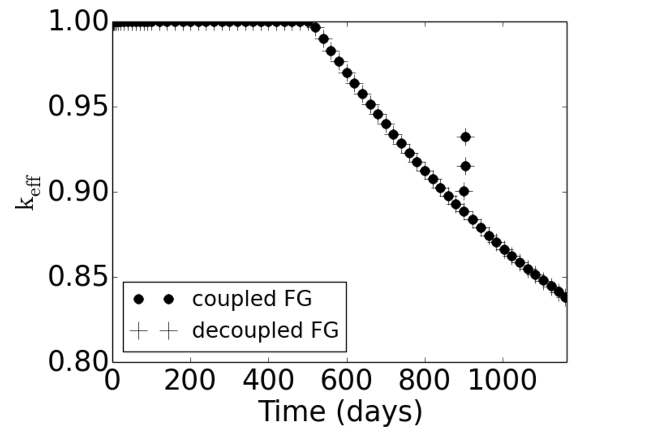

Fig. 6: The neutron transport eigenvalue (k_{eff}) for the pin array problem, comparing coupled and decoupled fission gas results.

Figure 7 shows the variation in pin power in the hottest and coldest fuel pins in the pin array. The shutdown is visible at $t = 900$ days, with two data points at about half the full power; these are the average power during one-hour ramps that bookend the 3.5 day shutdown. Figure 7 shows a very slight variation in the pin powers over the simulation time; the inter-pin power distribution was nearly fixed. The pin power difference was fairly steady and small at about 3000 W, but this was enough to cause a significant difference in the fission gas plenum inventory, as shown in Figure 8. At the end of the simulation, the hottest pin has 55% more fission gas in its plenum than the coldest pin; this shows that even small variations in pin power over a couple fuel cycles can have a significant effect on the plenum fission gas inventory. Also, Figure 8 shows a small burst in fission gas release during the shutdown, which is due to transient release. A higher power would result in more transient fission gas release during and immediately after the shutdown; in this case, fission gas coupling would become more significant.

V. CONCLUSIONS

The objective of this work was to develop and investigate a full-physics, consistent fission gas coupling method using MPACT and BISON. The MOOSE application Redwing was developed and used to perform a series of single- and multi-pin fuel depletion simulations. The results suggest that two-way coupled simulations can improve the prediction of fission gas behavior and other important quantities. A comparison of coupled and decoupled fission gas cases shows that fission gas coupling results in significant differences in the prediction of fission gas released, as well as smaller effects on other

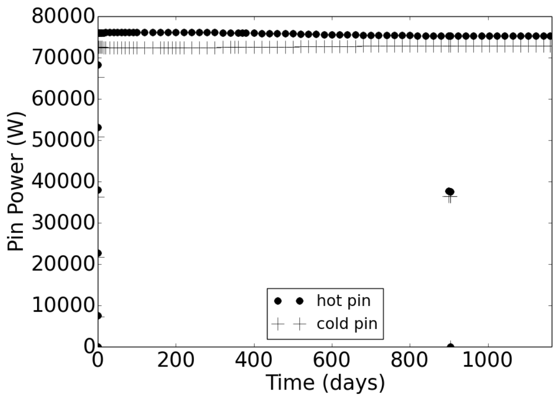

Fig. 7: This is a comparison of the hottest and coldest pin powers for the pin array simulation; fission gas coupling had an insignificant effect on the pin power distribution.

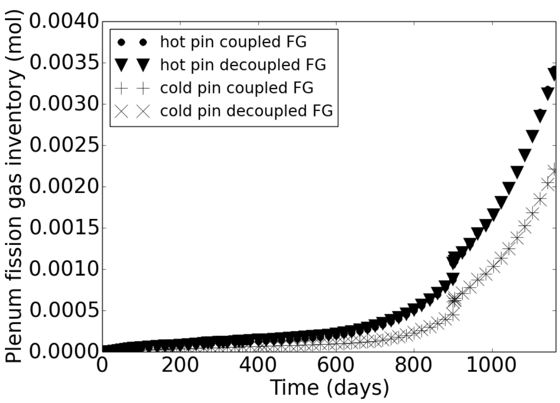

Fig. 8: This is a comparison between coupled and decoupled fission gas cases of the plenum fission gas inventory for the pin array simulation; results for the hottest and coldest pins are shown.

fission gas and non-fission gas quantities. The results suggest fission gas coupling can cause significant improvements in the solution for high-power and high-burnup cases.

There were several issues with the Redwing models which should be investigated. Cladding lift-off was predicted too early; more research is required to determine the specific causes of this. Also, the time step sensitivity suggests that there is a time-integration error, even at small Redwing time steps of a few days. This is likely due to using loose fission gas coupling along with MPACT's internal depletion solver.

There are several avenues for future modeling and simulation with fission gas coupling. The first is to perform a detailed, single- and multi-pin time step sensitivity study during and immediately after a shutdown event. For this new study, it would be important to perform higher-power simulations with shutdowns. According to BISON's Sifgrs model, a rapid decrease from a high fuel temperature results in a large transient fission gas release; with rapid fission gas release, fission gas coupling would become more significant. The pin array simulation results in Section IV. 3. suggest that fission gas coupling is only mildly important for modeling shutdowns, but in that case the pre-shutdown power and temperature were too low to result in significant transient fission gas release. In order to perform higher-power simulations, it is necessary to resolve issues fuel pin array model so that the BISON solver is able to handle problems at above 110% power. Two other cases in which fission gas coupling would be more significant are a case with a large amount of fission gas release before gap closure and a case with realistic clad lift-off, so that thermal neutrons streaming from the coolant to the fuel would cause more transmutation. Beside these simulations, work is currently underway to validate Redwing with Halden experimental data.

APPENDIX

Algorithm 1 details the method used to couple MPACT and BISON with Redwing, with a focus on fission gas-related quantities. The algorithm is based on the capabilities and limitations of MPACT and BISON, but it can be simplified by expressing it without referencing the individual programs and their meshes. It may be helpful to note which code corresponds to each step of the algorithm: steps 1-5 are MPACT, 6-10 are BISON, 11-13 are Redwing, and 14-23 are MPACT. Most steps are performed by `Coupler_Redwing` code (which is part of MPACT), although the Redwing executioner has top-level control.

Step 10 shows a balance equation for incremental fission gas release; while true, this is a stand-in for the much more complex Sifgrs algorithm, which calculates the incremental fission gas release based on a grain face bubble saturation criterion [3]. Steps 14 and 15 refer to the initial volumes of the gap and upper and lower plena; this is because MPACT's mesh remains undeformed throughout a Redwing simulation, so fission gas number density must be calculated based on undeformed volumes.

Also included in this appendix is Figure 9, which shows the runtime structure of Redwing during multi-pin simulations.

Algorithm 1 Fission gas (FG) coupling algorithm: continuous in space (no meshes)

Input: $\phi^{(i)}(\mathbf{r}, E), \mathbf{N}^{(i)}(\mathbf{r}), \mathbf{T}^{(i)}(\mathbf{r}), P^{(i)}, ...$

1: Solve the coupled neutron transport and nuclide transmutation equations:
$\phi^{(i+1/2)}(\mathbf{r}, E), \mathbf{N}^{(i+1/2)}(\mathbf{r}) = \mathrm{PC}(\phi^{(i)}(\mathbf{r}, E), \mathbf{N}^{(i)}(\mathbf{r}), \Delta t^{(i+1)})$

2: Compute intra-pin quantites for the coefficients of the thermomechanics problem:
$F(\mathbf{r}) = \int_0^\infty dE \Sigma_f(\mathbf{r}, E)\phi^{(i+1/2)}(\mathbf{r}, E)$
$q'''(\mathbf{r}) = \int_0^\infty dE \kappa \Sigma_f(\mathbf{r}, E)\phi^{(i+1/2)}(\mathbf{r}, E)$
$\phi_{fast}(\mathbf{r}) = \int_{1MeV}^\infty dE \phi^{(i+1/2)}(\mathbf{r}, E)$

3: Sum up FG nuclide number densities:
$N^{(i+1/2)}(\mathbf{r}) = \sum_{n=1}^{19} N_n^{(i+1/2)}(\mathbf{r})$ for $\mathbf{r} \in$ fuel

4: Compute incremental change in FG number density due to production and transmutation in fuel:
$\Delta N_{gen,tran}^{(i+1)}(\mathbf{r}) = N^{(i+1/2)}(\mathbf{r}) - N^{(i)}(\mathbf{r})$ for $\mathbf{r} \in$ fuel

5: Compute incremental change in FG number density due to transmutation in plenum:
$\Delta N_{tran}^{(i+1)}(\mathbf{r}) = N^{(i+1/2)}(\mathbf{r}) - N^{(i)}(\mathbf{r})$ for $\mathbf{r} \in$ plenum

6: Compute FG production rate:
$\beta^{(i+1)}(\mathbf{r}) = \Delta N_{gen,tran}^{(i+1)} / \Delta t^{(i+1)}$ for $\mathbf{r} \in$ fuel

7: **Simultaneously solve** thermomechanics problem, including FG release:

8: $\mathbf{T}^{(i+1)}(\mathbf{r}), V_{gap}^{(i+1)}, V_{plena}^{(i+1)} =$
$\mathrm{B}(\mathbf{T}^{(i+1)}(\mathbf{r}), F(\mathbf{r}), q'''(\mathbf{r}), \phi_{fast}(\mathbf{r}), N^{(i+1)}(\mathbf{r}), P^{(i+1)}, \Delta t^{(i+1)})$

9: Compute fuel FG number density field with Sifgrs:
$N^{(i+1)}(\mathbf{r}) = \mathrm{Sifgrs}(\mathbf{T}^{(i+1)}(\mathbf{r}), F(\mathbf{r}), \beta^{(i+1)}(\mathbf{r}), \Delta t^{(i+1)})$
for $\mathbf{r} \in$ fuel

10: Compute incremental FG release with Sifgrs:
$\Delta R = \int_{fuel} d\mathbf{r}(N^{(i)}(\mathbf{r}) + \beta^{(i+1)}(\mathbf{r})\Delta t^{(i+1)} - N^{(i+1)}(\mathbf{r}))$

11: Compute plenum FG inventory with no transmutation:
$P^{(i+1/2)} = P^{(i)} + \Delta R$

12: Compute gap FG inventory with deformed volumes:
$g^{(i+1)} = P^{(i+1/2)} V_{gap}^{(i+1)} / (V_{gap}^{(i+1)} + V_{plena}^{(i+1)})$

13: Compute upper/lower plena FG inventory with deformed volumes:
$p^{(i+1)} = P^{(i+1/2)} V_{plena}^{(i+1)} / (V_{gap}^{(i+1)} + V_{plena}^{(i+1)})$

14: Compute incremental change in FG number density in gap due to release:
$\Delta N_{rel}^{(i+1)}(\mathbf{r}) = g^{(i+1)} / V_{gap}^{(0)} - N^{(i)}(\mathbf{r})$ for $\mathbf{r} \in$ gap

15: Compute incremental change in FG number density in upper + lower plena due to release:
$\Delta N_{rel}^{(i+1)}(\mathbf{r}) = p^{(i+1)} / V_{plena}^{(0)} - N^{(i)}(\mathbf{r})$
for $\mathbf{r} \in$ upper and lower plena

16: Sum incremental changes in FG number density to get FG number density in plenum:
$N^{(i+1)}(\mathbf{r}) = N^{(i)}(\mathbf{r}) + \Delta N_{tran}^{(i+1)}(\mathbf{r}) + \Delta N_{rel}^{(i+1)}(\mathbf{r})$
for $\mathbf{r} \in$ plenum

17: Integrate FG number density field in plenum to get plenum FG inventory:
$P^{(i+1)} = \int_{plenum} d\mathbf{r} N^{(i+1)}(\mathbf{r})$

18: **for** $n = 1, X$ **do**

19: $f_n = \int_{fuel} d\mathbf{r} N_n^{(i+1/2)}(\mathbf{r}) / \int_{fuel} d\mathbf{r} N^{(i+1/2)}(\mathbf{r})$

20: Extend FG number density to nuclides in plenum based on fuel nuclide fractions:
$N_n^{(i+1)}(\mathbf{r}) = N_n^{(i+1/2)}(\mathbf{r}) + \Delta N_{rel}^{(i+1)}(\mathbf{r}) f_n$ for $\mathbf{r} \in$ plenum

21: **for** $n = 1, X$ **do**

22: Extend FG number density to nuclides in fuel based on local nuclide fractions:
$N_n^{(i+1)}(\mathbf{r}) = N^{(i+1)}(\mathbf{r}) N_n^{(i+1/2)}(\mathbf{r}) / N^{(i+1/2)}(\mathbf{r})$ for $\mathbf{r} \in$ fuel

23: Solve neutron transport problem again to account for feedback:
$\phi^{(i+1)}(\mathbf{r}, E) = \mathrm{Eigen}(\phi^{(i+1/2)}(\mathbf{r}, E), \mathbf{N}^{(i+1)}(\mathbf{r}))$

Output: $\phi^{(i+1)}(\mathbf{r}, E), \mathbf{N}^{(i+1)}(\mathbf{r}), \mathbf{T}^{(i+1)}(\mathbf{r}), P^{(i+1)}, ...$

where:

- $\mathbf{r}$ is the position vector.
- E is the neutron energy.
- $\Delta t^{(i+1)}$ is the time step from $t^{(i)}$ to $t^{(i+1)}$.
- ϕ is the scalar flux.
- $\mathbf{N}$ is the fission gas nuclide density field, indexed by nuclide n.
- PC is the MPACT solver operator, which solves coupled neutron transport and nuclide transmutation (P.C. stands for predictor-corrector)
- F is the fission rate density.
- q''' is the power density.
- κ is the energy released per fission.
- Σ_f is the macroscopic fission cross section.
- ϕ_{fast} is the fast neutron flux.
- N is the fission gas density field summed over all nuclides.
- $\Delta N_{gen,tran}$ is the change in fission gas number density due to generation and transmutation.
- ΔN_{tran} is the change in fission gas number density due to transmutation.
- $\mathbf{T}$ is the thermomechanics solution, which is comprised of intra-pin temperature and displacement fields.
- V_{gap} is the volume of the fuel/cladding gap.
- V_{plena} is the volume of the fuel/cladding upper and lower plena.
- B is the BISON solver operator, which solves the thermomechanics problem, yielding $\mathbf{T}$.
- Sifgrs is the Sifgrs operator, which updates the fission gas field; it is separated from B for clarity.
- X is the number of fission gas nuclides (this is 19 for the depletion library used in this study).
- Eigen is the operator which yields the solution to the neutron transport eigenvalue problem.

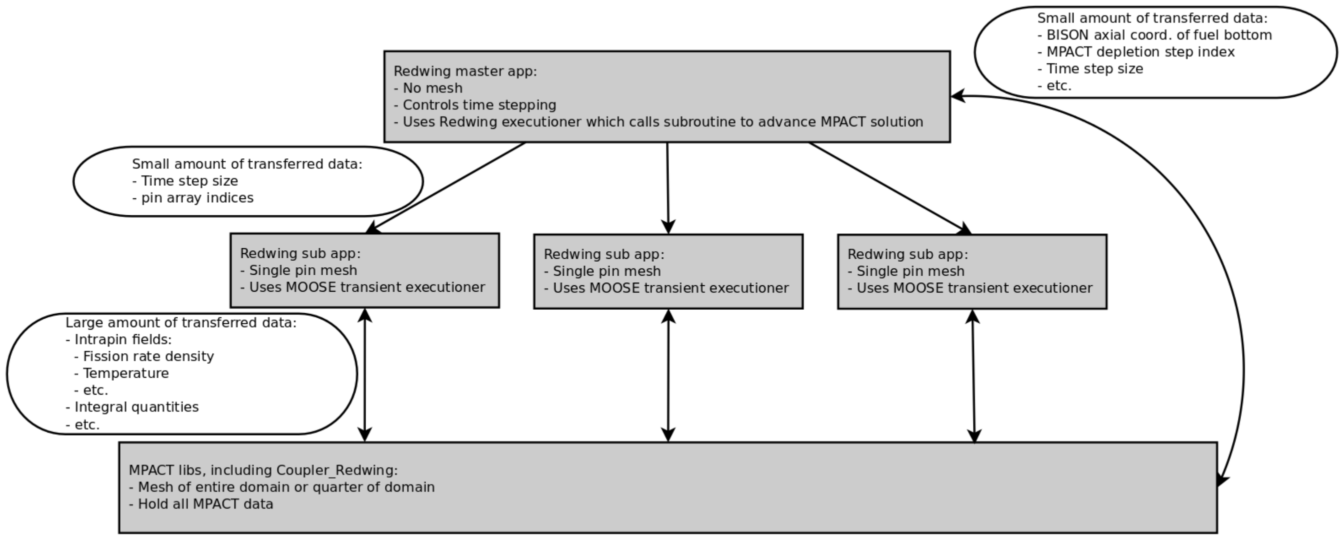

Fig. 9: This is the runtime breakdown of Redwing for a multi-pin simulation using MOOSE's `MultiApps` system. There is a master app, which runs the Redwing executioner, and there is one sub app for each fuel pin in the model, which corresponds to a BISON fuel pin mesh. The number of sub apps is the same as the number of BISON pins and MPACT pins.

ACKNOWLEDGMENTS

The authors would like to thank the MPACT, MOOSE, and BISON development teams for their help on numerous occasions during the development of Redwing. This material is based upon work supported under an Integrated University Program Graduate Fellowship. The fellowship is provided by the DOE. This work has also been supported by a Nuclear Regulatory Commission fellowship.

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