Coupling RELAP5-3D to BISON

A Step toward Coupled LOCA Analysis

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ABSTRACT

This report details two approaches for coupling the BISON nuclear fuel performance code with RELAP5-3D. Both approaches are shown to work well. The first is a Python-based approach, and the second combines the two applications into one executable with data passed in memory from one library to the other. This second coupling approach forms the basis for analysis of complex loss of coolant scenarios and enables future calculations of modeling uncertainties.

SUMMARY

Electric Power Research Institute and Idaho National Laboratory are partnered in developing a new tool for modeling loss of coolant accident conditions. This tool is based on the BISON nuclear fuel performance code and RELAP5-3D. BISON will compute the mechanical response of the fuel and cladding as well as the heat generated by the fuel. RELAP5-3D will compute the thermal-hydraulic conditions, including coolant temperatures and heat transfer characteristics.

The first approach in coupling these codes is based on a Python capability from within RELAP5-3D. This approach is viable but slower than desired. It has proven to work well, converging within three iterations for a steady-state case. Predictions are also good for a loss of coolant accident case.

The second approach is to couple these codes by passing data directly between them in a single executable. This required considerable modifications to RELAP5-3D. This approach also demonstrated good results, with calculations based on RELAP5-3D alone very closely matching those based on the new coupled tool.

Future work includes further verfication and validation and an assessment of performance from the perspective of best estimates and uncertainties.

ACKNOWLEDGMENTS

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ACRONYMS

DOE	United States Department of Energy
EPRI	Electric Power Research Institute
INL	Idaho National Laboratory
LOCA	loss of coolant accident
TCF	Technology Commercialization Fund

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Coupling RELAP5-3D to BISON

A Step toward Coupled LOCA Analysis

1. INTRODUCTION

Potential higher burnup fuel limits and the behavior of higher burnup fuel in loss of coolant accident (LOCA) conditions is of interest to the U.S. nuclear industry, including the Electric Power Research Institute (EPRI). Idaho National Laboratory (INL) and EPRI are partners on a United States Department of Energy (DOE) Technology Commercialization Fund (TCF) project to improve modeling of LOCA conditions for light water reactor fuels. The project aims to couple the BISON fuel performance code with the RELAP5-3D thermal hydraulic code. One of the major tasks of this project is to develop the specific coupling technology that will allow these two packages to communicate with one another. Details of this endeavor are the subject of this report.

Two approaches were taken for this coupling. The first is a Python-based technology from RELAP5-3D. This approach works, as will be shown, but it is limited in its usefulness due to its relative inefficiencies. The second approach is a so-called memory-based approach. In this approach, data is passed between the codes in memory, and the two codes operate as a single executable.

The sections that follow provide details of the approaches and give examples showing that both approaches accomplish the goal of coupling BISON and RELAP5-3D.

2. PYTHON-BASED COUPLING

A Python-based coupling between RELAP5-3D and BISON has been developed to explore the feasibility and effectiveness of integrating these two advanced simulation tools. Utilizing its Python-based interface, RELAP5-3D facilitates coupling with Computational Fluid Dynamics (CFD) tools such as STAR-CCM+ and OpenFOAM. This interface has now been extended to be compatible with the MOOSE (Multiphysics Object Oriented Simulation Environment) framework.

The main achievements in this coupling demonstration are:

- Demonstration of RELAP5-3D to BISON coupling for steady-state conditions in a typical Pressurized Water Reactor (PWR) model. The model includes the primary components of a PWR primary loop: pumps, downcomer, lower plenum, core, primary piping, pressurizer, and the primary side of the steam generator, with a fixed temperature used to model the secondary side.
- Demonstration of RELAP5-3D to BISON coupling during a large-break Loss-of-Coolant Accident (LOCA) event, encompassing phases such as blowdown, accumulator injection refill, and core reflooding.
- Implementation of iteration acceleration methods during LOCA transients to enhance the convergence rate per timestep in the Picard iterations between the codes.

The coupling methodology adopted for RELAP5-3D and BISON is depicted in Figure 1. The detailed coupling process is described in the following paragraphs.

From the RELAP5-3D calculations, the cooling of the hot channel is computed. Two alternatives were evaluated for passing RELAP5-3D information to BISON: First, passing the equivalent heat transfer coefficient

$h_c(z)$ and equivalent temperature $T_c(z)$. In this approach, the multiple heat transfer coefficients computed by RELAP5-3D (single-phase, boiling, critical heat flux, condensation, interfacial, and radiative heat transfer coefficients) are condensed into a single heat transfer coefficient, and the equivalent temperature $T_c(z)$ is fitted to preserve the axial heat flux. Second, providing BISON with the average wall heat flux computed by RELAP5-3D in coarse axial cells $q_r''(z)$, along with detailed pitching factors for the heat flux $f_p(z)$ and the wall temperature $p(z)$. This second approach reduces the need to post-process the heat transfer coefficients but showed issues with artificial aliasing due to axial conduction of heat in the cladding modeled by BISON but not accounted for by RELAP5-3D. This led to inaccuracies during the reflooding phase. Consequently, the first methodology was adopted.

From the BISON calculations, the wall displacement averaged over the azimuthal angle as a function of height $\langle d(z)\rangle_\theta$ and the exiting wall heat flux from the fuel rod averaged over the radius and azimuthal angle $\langle q''(z)\rangle_{r,\theta}$ are obtained. The displacements computed by BISON are used to update the area and hydraulic diameters of the axial nodes in the hot channel in RELAP5-3D. The averaged heat flux is imposed on the channel heat structures in RELAP5-3D to accurately model the temperature at the heat structure.

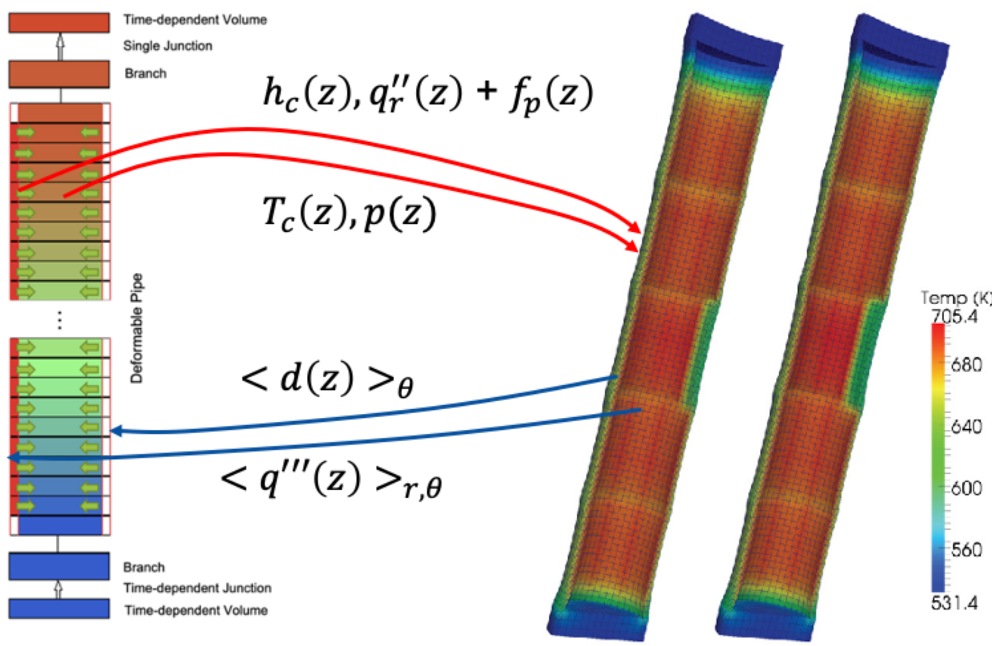


Figure 1. Coupling methodology between RELAP5-3D and BISON via RELAP5-3D's Python Interface.

The RELAP5-3D model of the PWR used for this demonstration is shown in Figure 2. This model represents a 4-loop PWR, where one loop is explicitly modeled, and the other three loops are lumped into an equivalent loop. The model includes the pump, low- and high-pressure accumulators, downcomer, lower plenum, average and hot channels in the core, upper plenum with remixing with downcomer inlet flow, pressurizer, and the primary side of a U-tube steam generator with an upper plenum. The core hot channel, which is coupled with BISON, is shown in further detail.

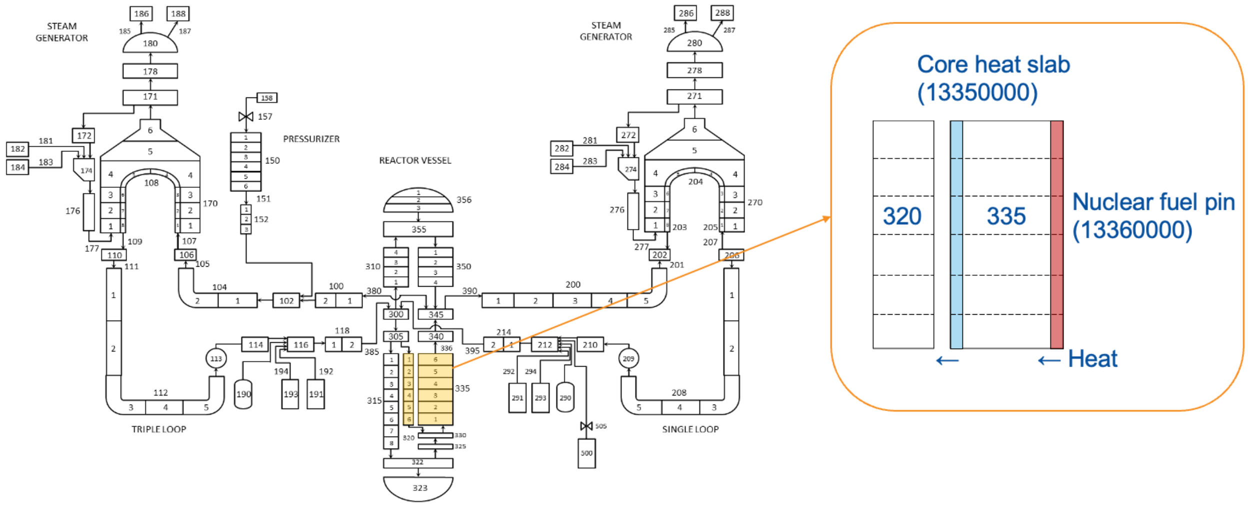
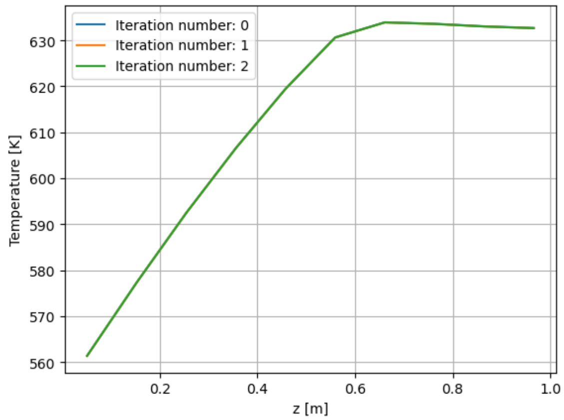
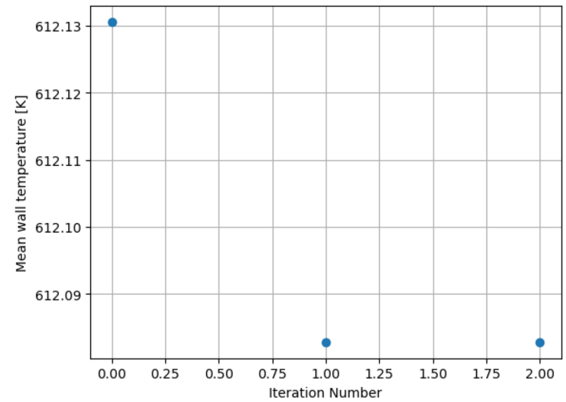


Figure 2. Nodal diagram for the PWR model used for demonstrating the coupling. The coupling occurs in the core hot channel, as highlighted in the figure.

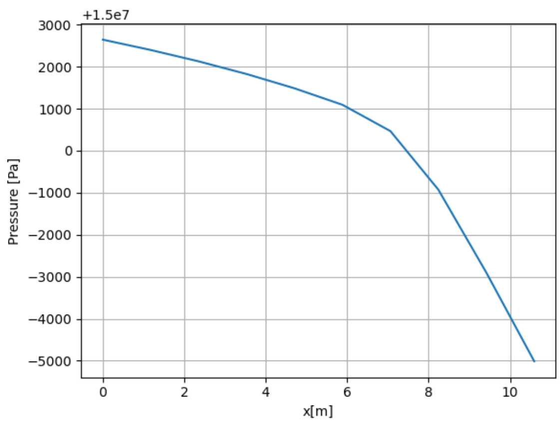
The results for steady-state operation are presented in Figure 3. The temperature rises to saturation as the flow moves up through the core. Pressure drops in the downcomer, followed by a significant pressure increase as the flow enters the core. Rod displacement follows the temperature field, with small thermal displacements observed due to thermal hoop stresses in the rod. However, these displacements are minimal. Additionally, the heat flux redistribution in the pin due to axial heat conduction modeled in BISON is small compared to the radial outlet heat flux from the pins. These small displacements and minimal heat redistribution result in the coupled system converging with a relative tolerance of transferred fields of 10^{-5} in three iterations.



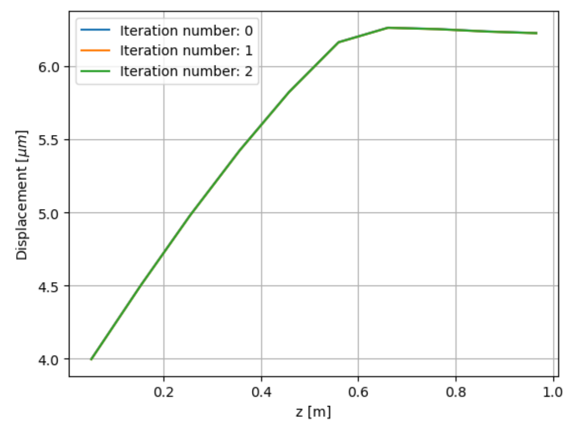
(a) Axial temperature as a function of height from the center of the core.



(b) Mean temperature for the hot channel as a function of iteration number.



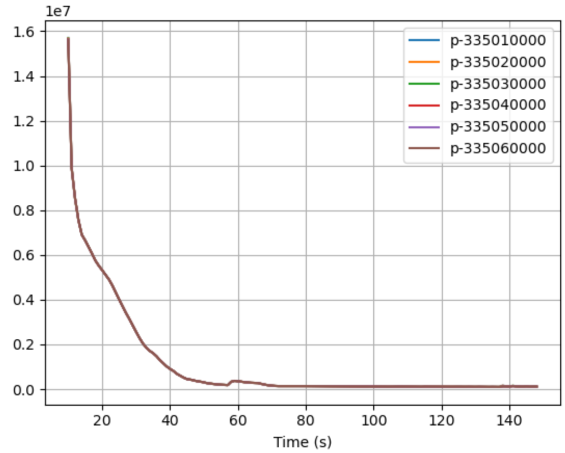
(c) Pressure across the core as a function of distance from the inlet to the downcomer.



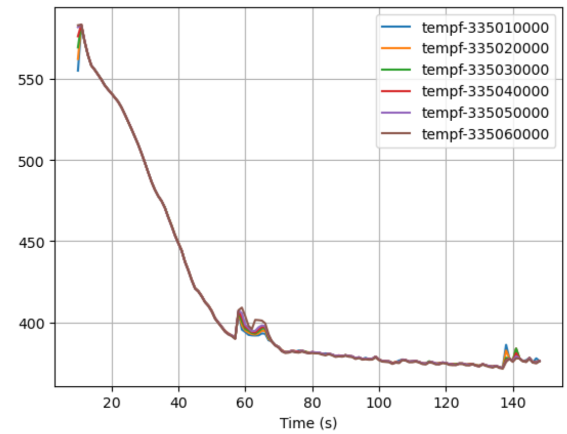
(d) Rod displacement from the bottom of the core as a function of iteration number.

Figure 3. Results of steady-state coupling for a typical PWR model.

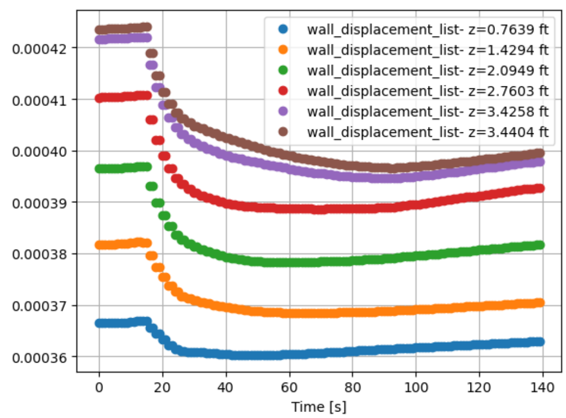
Following the development of the steady-state model, a large-break LOCA transient was simulated. The evolution of the average hot channel pressure and temperature during this transient is shown in the top panels of Figure 4. These phenomena exhibit the expected patterns of depressurization, refill, and reflood during the LOCA transient. The averaged wall displacements at different axial nodes from the bottom of the core are shown in the bottom panel of Figure 4. Initially, the rods balloon due to rapid depressurization and high fuel temperature. The displacement increases during the dryout phase as the fuel heats up further. This displacement gradually reduces as the core is flooded by the high-pressure accumulators.



(a) Pressure [Pa] as a function of time during the LOCA transient.



(b) Mean temperature [K] across the core as a function of time during the LOCA transient.



(c) Rod displacement [m] at different axial nodes as a function of time during the LOCA transient.

Figure 4. Results of the LOCA transient simulation. The top panels show the pressure and mean temperature as a function of time. The bottom panel shows the rod displacement at different axial nodes.

3. MEMORY-BASED COUPLING

The RELAP5-3D code has been reformatted as a primary library that is used by the main program. This allows the different phases of the execution to be neatly packaged, i.e., initialization, transient setup, time-advancement, and transient close-out are separable pieces of code. This allows an external code to link to the library and implement the initialization and setup phases while syncing the time-advancement with that of the master program. To accommodate this library configuration, a number of modifications were made to the RELAP5-3D code base. They are:

- A module was created, `RELAP5_API`, which contains all the necessary external API subroutines.
- The Fortran standard-calls to get the command line arguments has been wrapped within the API-module. This selectively uses either the standard calls or the command line arguments loaded from an external source, depending on whether the library is linked or not. This essentially allows a memory-linked program, such as BISON, to inject command line arguments.
- An API subroutine, `initRELAP53D`, has been added to combine the initialization and transient setup phase. This provides MOOSE the capability of initializing a MOOSE `Problem`.
- An API subroutine, `advanceTransientToTime`, has been added that calls a portion of the transient control code within RELAP5-3D. This subroutine does not merely take a timestep, it can take as many timestep as needed to match the advancement time.
- An API subroutine, `finishTransient`, has been added to allow RELAP5-3D end-of-simulation processes to execute appropriately (especially the output file printing), as well as to free memory appropriately.
- Several other subroutines/functions have been created for utility:
  - `mapComponentID`, provides the RELAP5-3D data structure-ID for a component in the user input.
  - `getComponentTypeID`, provides the internal type-ID of a component.
  - `getComponentNumberOfVolumes`, provides the number of sub-volumes of a component.
  - `getComponentVolumeLengths`, provides the volume lengths of a component.
  - `getComponent1DDataArray`, provides an array of any data associated with a component, e.g., pressure, void fraction, temperature of the liquid/gas, flow velocity, etc.
  - `mapHeatStructureID`, provides the RELAP5-3D data structure-ID for a heat-structure in the user input.
  - `getHeatStructureNumberOfSubStructures`, provides the number of sub-structure of a heat structure.
  - `getHeatStructureLengths`, provides the length variable of each substructure of a heat structure.
  - `setHSGBoundaryTemperature`, sets either the inner/outer boundary temperature of a heat structure.
  - `getHeatStructure1DDataArray`, provides an array of any data associated with a heat structure, e.g., temperature, heat transfer coefficient, heat flux, etc.

3.1. MOOSE-wrapped input

Portions of the RELAP5-3D model can be mimicked within MOOSE using input language in the classical MOOSE-HIT-format. An example is shown below:

```
[RELAP53D]
    relap_input_file_base = RELAP_TH
    relap_tpfdir = "../"
    verbosity_level = 2

    [pipe103]
        type = RELAPHydroComponentMeshGenerator
        component_id = 103
        var_names_to_mirror = 'p rhof rhog tempf tempg
                               tsatt satt velf velg'
    []
    [hs1031i]
        input = pipe103
        type = RELAPHeatStructureMeshGenerator
        component_id = 1031
        face_side = 'inner'
        block_name = 'hs1031i'
        var_names_to_mirror = 'httemp'
        axial_offset = '0.62e-3 0.0 0.0'
    []
    [hs1031o]
        input = hs1031i
        type = RELAPHeatStructureMeshGenerator
        component_id = 1031
        face_side = 'outer'
        block_name = 'hs1031o'
        var_names_to_mirror = 'htc_total t_sink'
        relap_var_names_to_overwrite = 'httemp'
        axial_offset = '0.62e-3 0.0 0.0'
    []
[]
```

With the capability to transfer RELAP5-3D to/from MOOSE meshes in place, we can now leverage normal MOOSE tools to transfer or manipulate the RELAP5-3D data.

3.2. Coupling strategy

The general strategy for in-memory coupling is to couple to RELAP5-3D hydrodynamic components (i.e., pipes, single-volumes, etc.) via the RELAP5-3D heat structures. In this fashion the coupled code, in this case MOOSE/BISON, can simulate the heat conduction where RELAP5-3D provides the convective heat transfer boundary condition. This was implemented as follows. The heat flux at the boundary, q'', is given by

$$q'' = h_{eff}(T_w - T_{eff,bulk}), \tag{1}$$

where h_{eff} is the effective heat transfer coefficient, T_w is the wall temperature, and $T_{eff,bulk}$ is the effective bulk coolant temperature. T_w is implicitly provided by the heat conduction solver (i.e., MOOSE/BISON) whilst h_{eff} and $T_{eff,bulk}$ are computed by RELAP5-3D. The latter thermal-hydraulics involves quite a sophisticated process to account for multiphase flows, the effect of flow regimes and the presence of flow stratification (to name but a few).

In addition to heat transfer coupling, BISON can also compute ballooning of cladding which will effect coolant channel flow areas. These effects can be transferred and incorporated into RELAP5-3D, although we are still working to discover good ways to verify such effects.

3.3. Verification

Simple verification was performed by comparing RELAP-BISON results to RELAP-standalone results. To this end a simple coolant channel with a single fuel rod has been modelled with a cosine axial profile. Both single-phase and two-phase heat transfer was verified by using different rod powers, as shown in Figures 5 and 6. The results show excellent agreement, however, some aspects of mesh resolution might create unrealistic results in the RELAP-BISON case especially if the BISON mesh resolution is much finer than that of RELAP, creating sawtooth-like temperature distributions.

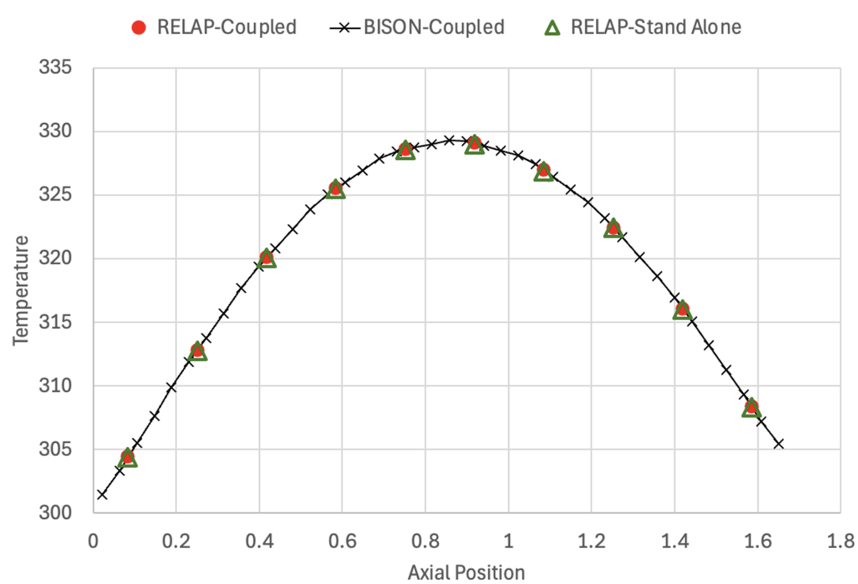


Figure 5. Steady simulation of RELAP-BISON and RELAP-standalone simulating a typical PWR fuel rod with a power of 4 kW. The results are cladding temperature versus fuel rod height.

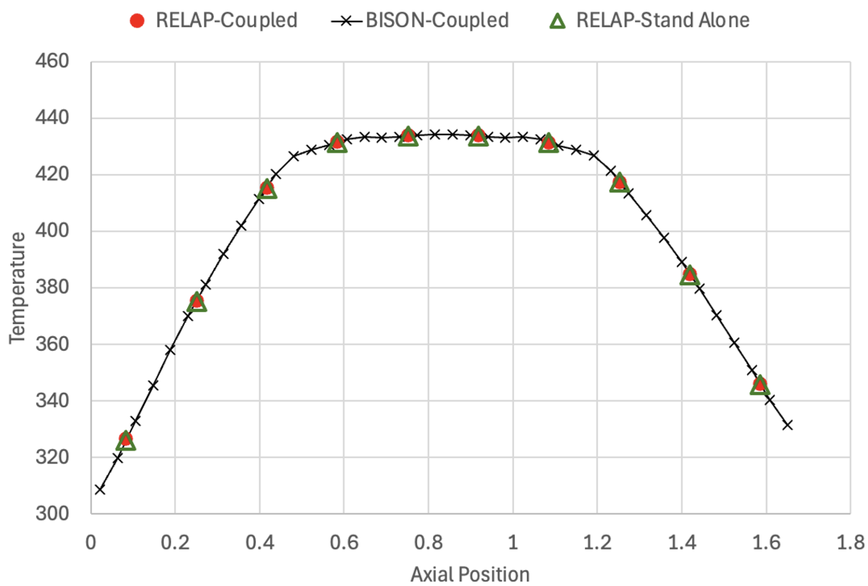


Figure 6. Steady simulation of RELAP-BISON and RELAP-standalone simulating a typical PWR fuel rod with a power of 24 kW. The results are cladding temperature versus fuel rod height.

Verification of transients has been performed by simulating a loss of flow transient to the same rod configuration. The results are shown in Figure 7 below.

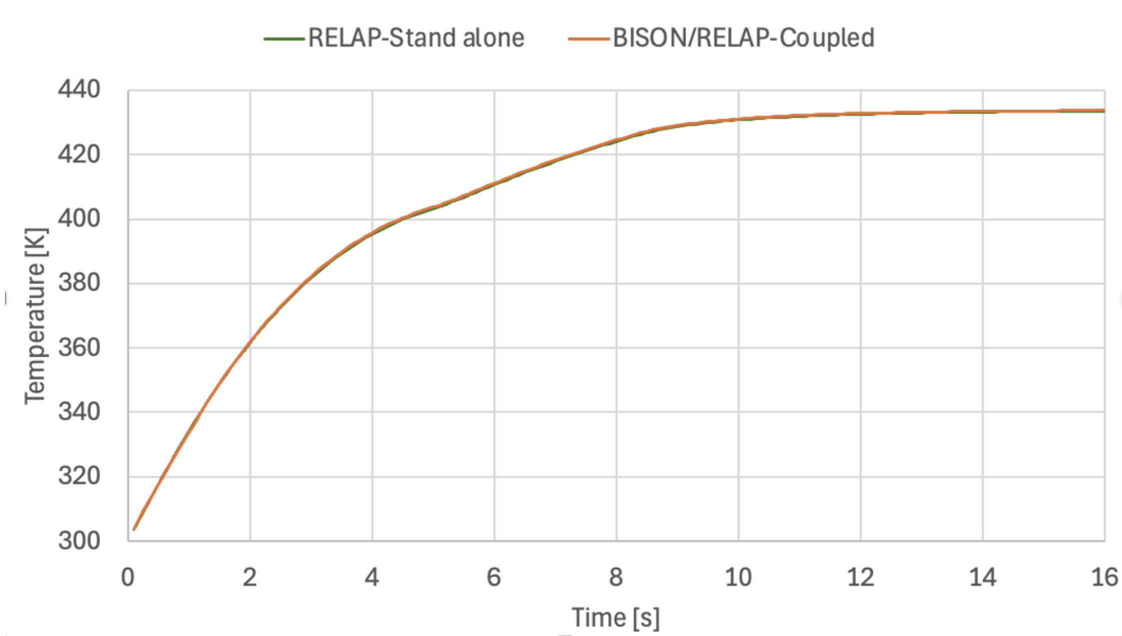


Figure 7. Transient simulation of RELAP-BISON and RELAP-standalone simulating a typical PWR fuel rod with a power of 24 kW. The results are centerline cladding temperature versus time.

3.4. Validation

For validation we plan on comparing both RELAP-BISON and RELAP simulations of a model of the famous LOFT L2-5 case. The thermal-hydraulic validation can be done using several parameters. One example of which, the upper plenum pressure, is shown in Figure 8 below.

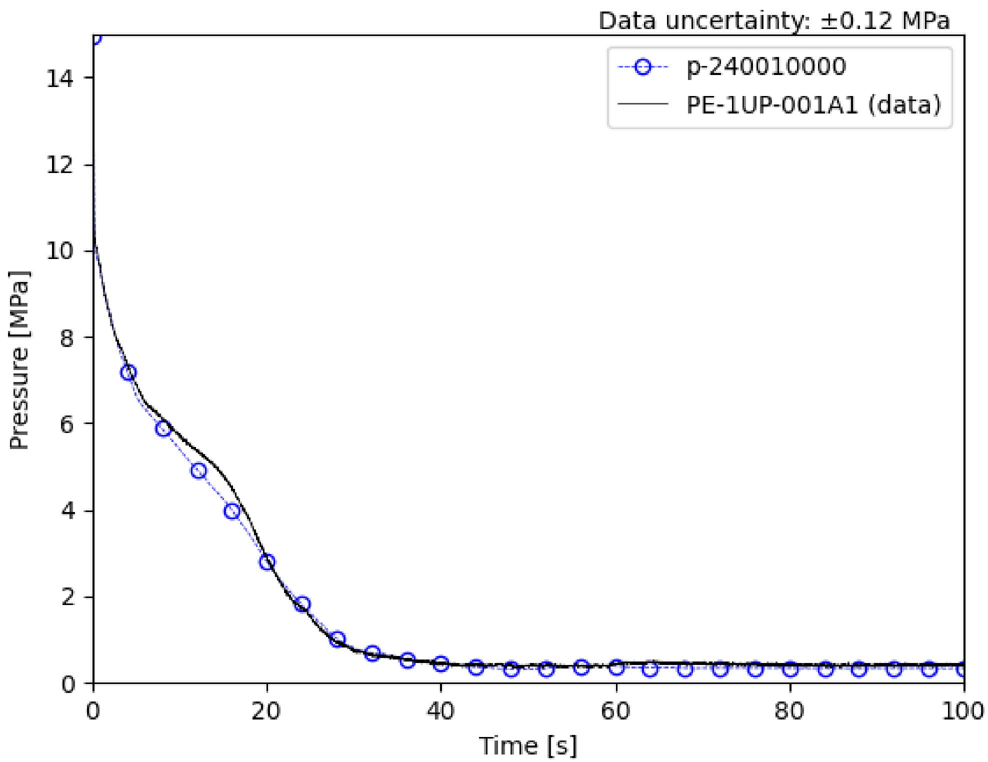


Figure 8. Transient simulation of the LOFT L2-5 case using RELAP-BISON showing the upper plenum pressure versus time.

Fuel temperature validation can be done via the many in-rod thermocouple measurements. An example is shown in Figure 9 below.

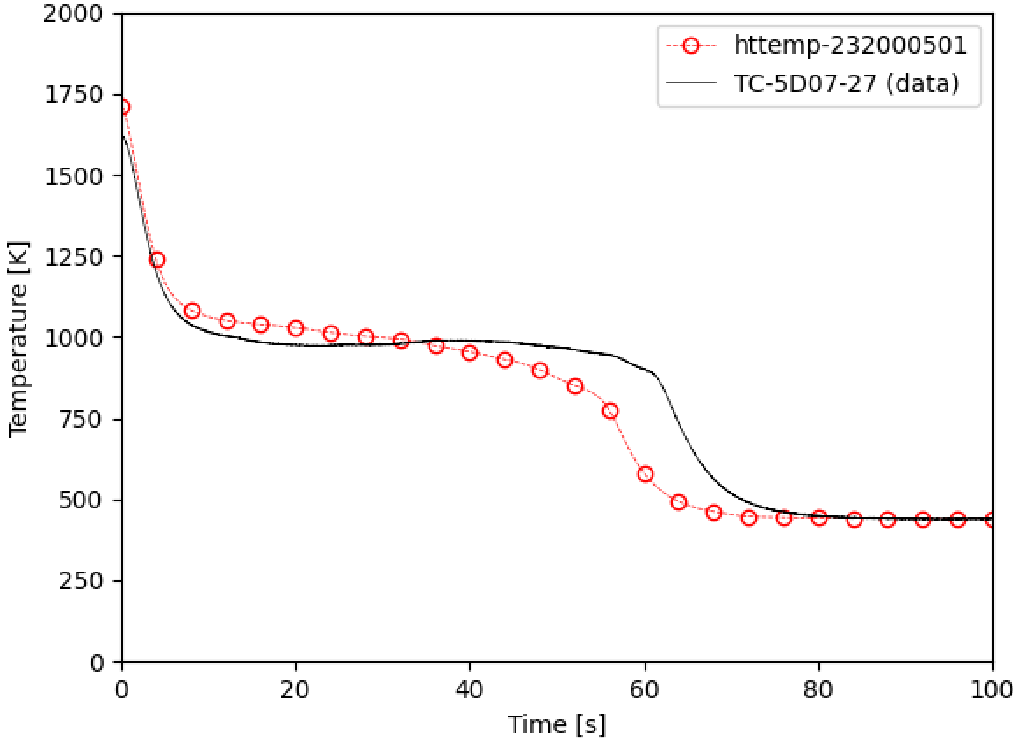


Figure 9. Transient simulation of the LOFT L2-5 case using RELAP-BISON showing fuel centerline temperature versus time, measurement taken 0.69 m above the bottom of the fuel rod.

More validation work is still required to ascertain whether the stress phenomenon is accurately captured, for which we may need different experimental data.

4. CONCLUSIONS

The Python-based coupling of BISON and RELAP5-3D works by sending a heat transfer coefficient and coolant temperature from RELAP5-3D to BISON and sending displacements and heat flux from BISON to RELAP5-3D. This is done via pre-existing mechanisms in RELAP5-3D. In this approach, the codes communicate information but execute as stand-alone applications.

The Python-based coupling was implemented first as it was the most straightforward approach. It is a relatively inefficient approach as data is not transferred directly between the codes but indirectly through files. Nevertheless, it has shown itself to be robust, with only three Picard iterations required for convergence at a given step for a steady-state case. Results from a LOCA case are also well behaved.

The memory-based coupling is more efficient since data is transferred between the codes directly. In this case, the two codes operate as a single application. This capability required considerable adjustments to RELAP5-3D, including creating a new module to house the external-facing application programming interface and developing a number of utility routines. One advantage of this work is that these routines may be used to couple RELAP5-3D to any MOOSE-based application.

The memory-based coupling approach was shown to give good results. Results from a RELAP5-3D standalone calculation of a simple fuel rod compared very well to results from a coupled calculation. Results from a LOFT L2-5 case showed good quality as well.

The memory-based coupling approach will be exercised further in the final months of this project. More validation work will occur. This will enable evaluation of best estimate accuracy and uncertainty quantification. These results will be presented in a final report, which will include a review of all the activities of the project. At the conclusion of the project, the coupled code will be available for use by the broader nuclear engineering community.