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Oak Ridge National Laboratory Coupling of CTF and TRACE for Modeling of Transients

A. Wysocki
R. Salko
B. Collins

June 30, 2021

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A. Wysocki R. Salko B. Collins

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ABBREVIATIONS

BC boundary condition

CASL Consortium for Advanced Simulation of Light Water Reactors

CFL Courant-Friedrichs-Lewy

ECI Exterior Communications Interface

HDF5 Hierarchical Data Format 5

MPACT Michigan Parallel Characteristics Transport Code

MSIV main steam isolation valve

MSLB main steam line break

NRC US Nuclear Regulatory Commission

PWR pressurized water reactor

RCP reactor coolant pump

SNAP Symbolic Nuclear Analysis Package

T/H thermal hydraulics

TRACE TRAC/RELAP Advanced Computational Engine

XML Extensible Markup Language

ABSTRACT

This report documents the improvements that have been made to the capabilities for coupling CTF to systems codes, specifically the US Nuclear Regulatory Commission TRAC/RELAP Advanced Computational Engine (TRACE) code. An initial systems coupling capability was set up previously by using a nonoverlapping domain approach with the codes exchanging data at the core boundaries. The present work adds a new approach by using overlapping domains in which the system code also models the core. A new input format was added to allow users to specify the physical quantities to be exchanged and their location in the system model, which gives the flexibility of applying one-way or two-way coupling between the codes by using the desired data exchanges. In addition to applying thermal hydraulics boundary condition values obtained from TRACE, a capability was added to allow CTF to apply flow resistance feedback to TRACE to match the CTF core pressure drop. Support was added for executing parallel CTF models within the CTF system's coupling. The system coupling capability was successfully applied to a parallel main steam line break transient, demonstrating that both the one-way and two-way coupling behaved as expected and provided substantial improvements to numerical stability and run time compared with the previous nonoverlapping domain coupling. An initial capability was also developed for performing restart calculations in CTF, which will be used in the future for restarting CTF-TRACE simulations at specific points in the transient simulation.

1 INTRODUCTION

An initial capability to couple CTF to a systems code was implemented in the Consortium for Advanced Simulation of Light Water Reactors (CASL) milestone L3:PHI.TRN.P19.01 (Wysocki et al. [2019]). In that work, CTF was coupled to the US Nuclear Regulatory Commission (NRC) thermal hydraulics (T/H) systems code TRAC/RELAP Advanced Computational Engine (TRACE) by using a nonoverlapping domain approach with explicit coupling. The communication between codes was achieved with the Exterior Communications Interface (ECI), which is provided as either a stand-alone or built-in utility with TRACE.

In the explicit, nonoverlapping domain coupling approach, only CTF modeled the core region. The TRACE model included the remainder of the system and applied the core conditions from CTF—outlet temperature, outlet flow rate, and inlet pressure—as core inlet and outlet boundary condition (BC) values at each time step. This approach provided an easy-to-implement, initial two-way coupling method between the two codes. This coupling method was found to require very small timestep sizes due to the numerical stability considerations discussed below. At that time, a more sophisticated implicit coupling had been envisioned for future work in order to improve the stability and runtime of the coupling. The present work achieved this goal instead by employing an overlapping domain coupling approach that is described afterward.

Previous studies (Weaver et al. [2002], Soler-Martinez [2011]) state that explicitly coupling two T/H codes across separate physical domains requires that the sonic Courant-Friedrichs-Lewy (CFL) remain below unity to ensure the numerical stability of the momentum transport calculation. The CFL limit applies to the solution of fluid transport quantities (e.g., density, enthalpy, pressure) that are solved with an explicit numerical scheme (i.e., when the current time step values are calculated from only the previous time step values in the same cell and neighboring cells). Because the current time step values are based only on the nearest adjacent upwind cell for first-order upwind schemes, as in CTF, transported quantities that travel more than one cell length in a given time step will result in an unstable solution. The CFL imposes a restriction on the time step size to prevent this from occurring.

When solving for density and enthalpy, the characteristic transport velocity is the material velocity of the fluid. When solving for pressure, the characteristic velocity is the speed of sound in the fluid, which is several orders of magnitude larger than the material velocity. For this reason, T/H codes, including CTF and TRACE, solve the pressure field implicitly (i.e., simultaneously in all cells in the solution domain in a given time step). This ensures that only the much less restrictive material CFL limit must be adhered to, although some numerical schemes can also remove this restriction.

However, even though CTF and TRACE each solve the pressure field implicitly, applying an explicit pressure coupling across the fluid interface between the code domains means that the entire solution could be unstable unless the sonic CFL limit is satisfied. As a result, the initial explicit nonoverlapping domain coupling implemented for CTF-TRACE was found to suffer from significant numerical stability issues and required extremely fine time step sizes well below the time step limit applicable to either code separately. For a full pressurized water reactor (PWR) system model, achieving steady-state coupled convergence required approximately 5,000 coupled CTF-TRACE iterations (i.e., 5,000 full CTF steady-state solves and 5,000 TRACE steady-state solves). A coupled transient simulation was not achieved with this full PWR model because of numerical instability. A transient simulation was instead performed with a single channel CTF model and a simplified single-loop system model, including a pump and heat exchanger. A hypothetical transient scenario was performed that perturbed the pump speed by +/- 10% of its nominal value. It was demonstrated that the correct T/H values were communicated and applied between the codes; however, even this simple transient required very small time step sizes and limited perturbation from steady-state conditions to complete the simulation successfully.

One possible route to improve the coupling is to implement an implicit solution of the pressure field across both domains—CTF and TRACE—simultaneously. Both codes use a similar general approach based on the Semi-Implicit Method for Pressure Linked Equations algorithm to solve the mass, momentum, and energy conservation equations (Salko et al. [2017], Bajorek et al. [2017]). Within the iteration scheme, the ECI allows for fairly fine-grained specification to designate the point at which data can be transferred between codes. This could allow implicit pressure coupling through the implicit iteration between the codes within a time step.

However, this approach could require significant CTF coding modifications to implement, and unforeseen complications could arise in the efforts to achieve truly implicit stable coupling with this method. Instead, a more straightforward and less intrusive approach was adopted in the present work in which TRACE solves the entire system, including the core, and exchanges core information with CTF to enforce consistency between the two solutions. As shown in this report, the new coupling approach provided greatly improved numerical stability and increased time step sizes compared with the original approach. The new coupling was able to model a challenging transient event with larger and more rapid perturbations over time compared with what was achievable with the previous coupling.

2 COUPLING IMPROVEMENTS

The milestone L3:PHI.TRN.P19.01 report (Wysocki et al. [2019]) provides details of the system coupling implementation within CTF, including the creation of a derived type, `SystemCoupling_type`, which is called during CTF solves and handles all necessary interaction with the ECI to send and receive TRACE data. It also calls the appropriate CTF routines to apply core-wide T/H BCs—inlet temperature, inlet flow rate, and outlet pressure—in the CTF model.

The coupling was set up to perform either steady-state or transient simulations, depending on the value of the steady-state flag (`notrans`) in the CTF input file. The calculation approach is as follows.

- For steady-state simulations, each code is run sequentially and repeatedly until the change in the coupled solution between coupled iterations is less than the specified coupled convergence tolerances. Each code run within a coupled iteration consists of a full steady-state solve until that code's steady-state convergence criteria are met. Data are exchanged between codes in between these stand-alone steady-state solves.
- For transient simulations, a steady-state solution is first achieved as described previously. Then, the transient time advancement proceeds in an explicit manner with the codes exchanging data at each time step. Both codes use the same time step size at each time step according to

  $$\Delta t = \min(\Delta t_{max,TRACE}, \Delta t_{max,CTF}), \quad (1)$$

  where Δt is the actual time step size used by both codes, and $\Delta t_{max,TRACE}$ and $\Delta t_{max,CTF}$ are the maximum allowable time step sizes determined by TRACE and CTF, respectively.

The current work retains this general solution approach while making the methodological and performance improvements described in the following sections.

2.1 OVERLAPPING DOMAIN COUPLING

As discussed in Section 1, the previous system coupling implementation used a nonoverlapping domain coupling approach in which the TRACE model does not include the core and calculates the system response by using CTF-provided core BCs (i.e., outlet flow rate, outlet temperature, and inlet pressure). TRACE in turn provides core inlet flow rate, inlet temperature, and outlet pressure BCs to the CTF core calculation.

The present work introduces an overlapping domain coupling approach in which TRACE models the entire system, including the core. Two overlapping domain options are explored in this work: (1) a one-way coupling in which TRACE passes the core inlet temperature, inlet flow rate, and outlet pressure BCs to CTF and CTF does not provide any values back to TRACE and (2) a two-way coupling identical to the one-way coupling except that CTF provides pressure drop feedback to TRACE to so that the TRACE effective core pressure drop matches CTF.

This pressure drop feedback is accomplished by adding a valve component in the TRACE model immediately upstream of the core. Such a valve does not exist in an actual PWR, but it serves a function numerically similar to a throttle or flow control valve by introducing an additional pressure loss to the primary loop flow path. In the current implementation, CTF calculates the valve flow area fraction (A/A_0)—where A_0 is the fully open flow area—that will produce the desired valve pressure drop equal to the difference in the CTF core pressure drop (ΔP_{CTF}) and the TRACE core pressure drop (ΔP_{TRACE}) at the current time step:

$$\Delta P_{diff} = \Delta P_{CTF} - \Delta P_{TRACE}. \tag{2}$$

By default, the valve frictional loss factor (K) is calculated by TRACE by using a built-in correlation, which is a function of (A/A_0) and the local valve flow conditions. However, an option is available to specify a user-defined relationship between K and (A/A_0). Any relationship would be acceptable for the current purposes if the same relationship is used in the TRACE model and CTF calculation of (A/A_0). For simplicity, a linear relationship was used:

$$K = K_0\left(1 - \frac{A}{A_0}\right). \tag{3}$$

The value of K_0 is arbitrary and must only be chosen so that it is large enough to give sufficient pressure drop feedback to bound the codes' pressure drop difference. A value of 100 was found to be sufficient for the current application. For a given K, the valve pressure drop is given by

$$\Delta P_{valve} = \frac{\rho_{valve} v_{valve}^2}{2} K, \tag{4}$$

where ρ_{valve} and v_{valve} are the fluid density and velocity, respectively, in the valve at the current time step.

By combining these equations, the valve area fraction corresponding to $\Delta P_{valve} = \Delta P_{diff}$ is:

$$\frac{A}{A_0} = \left(1 - \frac{2\Delta P_{diff}}{K_0 \rho_{valve} v_{valve}^2}\right). \tag{5}$$

TRACE must provide three quantities—ΔP_{TRACE}, rho_{valve}, and v_{valve}—to CTF at each time step for CTF to determine the valve area fraction to apply to TRACE.

One implication of this valve-based approach is that a larger percentage of the final core pressure drop in the TRACE model will be localized at the core inlet compared with the more evenly distributed pressure drop calculated in CTF. This will slightly impact the core axial pressure drop distribution. However, the total core pressure drop is the far more important parameter because of its impact on loop pressure dynamics and core flow rate; the local pressure distribution within the core will only impact local thermophysical fluid properties, and these are extremely insensitive to such small pressure variations, particularly for incompressible single-phase flow. Therefore, localizing the pressure drop at the core inlet minimally impacts the TRACE solution.

Another implication of the valve-based approach is that the valve can only add pressure drop to the TRACE model, not subtract it. This was not an issue in the current demonstration because the TRACE model exhibited a lower core pressure drop than CTF, so a positive ΔP_{diff} was needed. However, if TRACE predicted a higher pressure drop than CTF, this could be addressed by reducing or eliminating the grid loss factors from the TRACE model but not the CTF model. This would be a convenience for ensuring that the TRACE core pressure drop before CTF feedback correction is below the CTF core pressure drop so that a valve pressure drop can be added to match the total core pressure drop in both codes. This will impact the core axial pressure distribution, but for the aforementioned reasons, this impact is negligible given that the correct total core pressure drop will still be attained. A warning was added to the code to alert users if TRACE has calculated a higher core pressure drop than CTF, in which case an adjustment to the TRACE model might be required.

In future work, it might be possible to directly adjust the TRACE core friction or local loss factors within the core through the ECI rather than to use an artificial valve component below the core. It has not yet been determined whether such an adjustment is achievable through the ECI. Such an adjustment would more precisely match the distributed pressure drop behavior in both codes, which might produce more accurate results under two-phase core conditions and/or when a more finely discretized TRACE core model is used, in which case the axial pressure drop distribution in each channel might impact the TRACE-predicted cross flow. However, the present work only considers single-phase transient conditions and a single radial channel TRACE model; therefore, the valve-based approach is currently sufficient.

2.2 USABILITY

Previously, the types of data being transferred and their locations in the TRACE model were hard-coded into `SystemCoupling_type`. This included core inlet temperature, inlet flow rate, and outlet pressure from TRACE and core outlet temperature, outlet flow rate, and inlet pressure from CTF. All these quantities were required to be passed during coupled simulations, and the TRACE model was required to use the specific component and cell numbering at which the corresponding values would be sent and received.

To allow flexibility in coupling CTF to a variety of TRACE models—each with different component and cell numbering schemes—and flexibility in which quantities are to be exchanged, a capability was added to allow these specifications to be read from an input file. Currently, this is in the form of a separate input file using Extensible Markup Language (XML) format. An example snippet of such a file that replicates the original nonoverlapping domain coupling behavior is given in Figure 1, and one that defines a two-way overlapping domain coupling is given in Figure 2. In Figure 2, the CTF-to-system transfers `CoreOutletTemp`, `CoreOutletFlow`, and `CoreInletPres` are not provided in the XML file; therefore, these quantities are excluded from the coupling. Instead, in this case, `CoreInletPres`, `ValveDens`, and `ValveVel` are transferred from TRACE to CTF, and `ValveAreaFrac` is transferred from CTF to TRACE to provide the core pressure drop feedback, as discussed in Section 2.1.

An overlapping-domain approach with one-way (TRACE to CTF) coupling can be specified by eliminating the three parameters related to pressure drop feedback, resulting in only the three TRACE to CTF core BC parameters being applied.

The current CTF-TRACE coupling only supports the exchange of full-core T/H BCs between the codes. Future work will implement the ability to set radially dependent BCs so that each radial and azimuthal TRACE core channel will be coupled to the set of CTF channels in the corresponding region of the core. This will improve the modeling fidelity, particularly for transients such as main steam line break (MSLB), which exhibit large radial asymmetries due to the break occurring in only one loop while the other loops remain intact. Once this feature is available, the mapping of TRACE radial and azimuthal core channels to CTF channels will be performed through the coupling input file.

```
<ParameterList name="TRANSFER_POINTS">
  <ParameterList name="SYSTEM_TO_CTF">
    <ParameterList name="CoreInletTemp">
      <Parameter name="CompNum" type="int" value="20"/>
      <Parameter name="CellNum" type="int" value="7"/>
    </ParameterList>
    <ParameterList name="CoreInletFlow">
      <Parameter name="CompNum" type="int" value="20"/>
      <Parameter name="CellNum" type="int" value="7"/>
    </ParameterList>
    <ParameterList name="CoreOutletPres">
      <Parameter name="CompNum" type="int" value="21"/>
      <Parameter name="CellNum" type="int" value="1"/>
    </ParameterList>
  </ParameterList>
  <ParameterList name="CTF_TO_SYSTEM">
    <ParameterList name="CoreOutletTemp">
      <Parameter name="CtrlVar" type="int" value="-3"/>
    </ParameterList>
    <ParameterList name="CoreOutletFlow">
      <Parameter name="CtrlVar" type="int" value="-1"/>
    </ParameterList>
    <ParameterList name="CoreInletPres">
      <Parameter name="CtrlVar" type="int" value="-2"/>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Figure 1. Example XML input file defining a nonoverlapping domain coupling.

```xml
<ParameterList name="TRANSFER_POINTS">
  <ParameterList name="SYSTEM_TO_CTF">
    <ParameterList name="CoreInletTemp">
      <Parameter name="CompNum" type="int" value="22"/>
      <Parameter name="CellNum" type="int" value="1"/>
    </ParameterList>
    <ParameterList name="CoreInletFlow">
      <Parameter name="CompNum" type="int" value="22"/>
      <Parameter name="CellNum" type="int" value="1"/>
    </ParameterList>
    <ParameterList name="CoreOutletPres">
      <Parameter name="CompNum" type="int" value="21"/>
      <Parameter name="CellNum" type="int" value="1"/>
    </ParameterList>
    <ParameterList name="CoreInletPres">
      <Parameter name="CompNum" type="int" value="22"/>
      <Parameter name="CellNum" type="int" value="1"/>
    </ParameterList>
    <ParameterList name="ValveDens">
      <Parameter name="CompNum" type="int" value="50"/>
      <Parameter name="CellNum" type="int" value="2"/>
    </ParameterList>
    <ParameterList name="ValveVel">
      <Parameter name="CompNum" type="int" value="50"/>
      <Parameter name="CellNum" type="int" value="2"/>
    </ParameterList>
  </ParameterList>
  <ParameterList name="CTF_TO_SYSTEM">
    <ParameterList name="ValveAreaFrac">
      <Parameter name="CtrlVar" type="int" value="-111"/>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Figure 2. Example XML input file defining a two-way overlapping domain coupling.

2.3 PARALLELIZATION

The original coupling of CTF and TRACE only supported running serial CTF models. Because this capability ultimately must support running much larger, pin-resolved CTF models, it was necessary to add support for parallel CTF models to the capability. When implementing this capability, it was determined that TRACE will still a run on a single process only (i.e., the root processor) and that all communication with TRACE will occur on that process only. This means that all CTF solution data that must be passed to TRACE must first be reduced to root, and all TRACE solution data needed by CTF must be expanded to all processors. The `SystemCoupling` class was modified so that it is always called by all processors in the CTF message passing interface communicator. The required expansion or reduction of data before communication with TRACE is handled entirely within the class.

To test the capability, a small quarter symmetry five-assembly model (three actual modeled assemblies) with each assembly having 3×3 pins was created in CTF. Both serial and parallel (three processors) variants of the model were created. This case is run as a steady-state simulation coupled to TRACE by using both of the serial and parallel models. Upon completion of the simulations, the results files are compared with one another, and a diff is done to ensure that results match to within the testing tolerance. This test was added as an automated regression test that runs as part of the CTF regression testing matrix and ensures that this new feature continues to work as expected.

3 RESTART CAPABILITY

The coupled system capability will often require running long transients, which will require long job times on high-performance computing systems. To support this, a restart capability was implemented into CTF, which will allow users to instruct CTF to dump its solution data to a restart file, which can then be used to restart the code simulation from that save point.

The capability was designed to support two primary use cases: (1) stand-alone CTF shall be able to write restart data to a restart file and (2) CTF shall expose its restart data through the CTF coupling interface, which will allow a coupled code to obtain and set restart data on command. General requirements for the stand-alone use case are as follows.

- Restart data shall be written to a Hierarchical Data Format 5 (HDF5) file called `<name>.res_out.h5`, where `<name>` is the base name of the input file.
- Each restart save will be written to a separate group in the HDF5 file.
- An option will be made available in the CTF input deck that will allow users to specify that a restart file shall be generated.
- Users shall be able to choose intervals in the transient in which data shall be saved to the restart file.
- If users do not specify the restart dump interval, then a restart dump will be made at the end of the simulation by default.
- Users shall be able to specify that a restart file will be read by CTF.
- Users shall be able to specify from which group in the restart file CTF shall restart. If this is not specified, then CTF will restart from the last restart group in the file by default.
- The restart file shall be named `<name>.res_in.h5`, which will prevent overwriting the restart file if a new one is being generated by the CTF simulation.

The general requirements for the coupled capability are as follows.

- CTF shall provide a subroutine in the CTF coupling interface that, when called, will return three 1D vectors—string, integer, and float data—for the fluid solution. The vectors shall contain all the data CTF needs to perform a restart.
- CTF shall provide a subroutine in the CTF coupling interface that will accept the three 1D vectors obtained from the fluid restart data `get` procedure. CTF shall use the provided data to initialize the solution.
- CTF shall provide a subroutine in the CTF coupling interface that, when called, will return three 1D vectors—string, integer, and float data—for a single pin in the model.
- CTF shall provide a subroutine that accepts the three 1D restart vectors provided by the pin restart data `get` subroutine, which will be used to initialize the pin solution.
- CTF shall provide coupling interface procedures that allow the driver code to direct CTF to write a save point to its restart file, as well as to direct CTF to read a save point from its restart file and use that to initialize the CTF solution. This option differs from the previous ones because the driver code

is not responsible for managing the restart data because the restart data are stored in the native CTF restart file.

A separate set of interface procedures is provided for handling pin restart data to allow the coupled code to shuffle the fuel pins during the restart. A similar feature is not provided for channel data because additional complexity is involved in determining which channels belong to which assemblies in the model. Therefore, the shuffling capability is only meant to be used for depletions, in which case the channel solution restart data are not important because there is no history effect and only steady-state simulations are being performed. The general requirements shared by both capabilities are as follows.

- The model geometry (e.g., number of channels, pins, gaps, channel geometry, pin geometry) shall not change between the model that generated the restart data and the model that is reading the restart data. Modeling options and BCs can be changed via the input file after a restart.
- The restart capability shall support running parallel CTF models.

To help meet the aforementioned requirements, a new class was developed for storing key/value pairs of data needed to do the restart, which was named the `DataBase` class. This class performs several functions to meet requirements, including:

- accepting scalar and array data and an associated data tag (i.e., key) that can be used to retrieve that data;
- storing data in a hierarchical format, which allows nesting of `DataBase` objects;
- providing method for reducing parallel data to root for exchange with other codes or writing to the restart file;
- collapsing the database into a set of string/integer/float vectors suitable for sending to the coupled code or writing to the restart file; and
- reconstructing the database from the raw data vectors that were generated by the `DataBase` class.

The `DataBase` class allows each class in CTF that has data needed in the restart to construct its own `Database` object, which is returned to the caller. The actual class data may remain private. Because `DataBase` objects can be nested, subclass `DataBase` objects can be added to the `DataBase` object that owns the subclass. Because all data are tagged, when a class receives a `DataBase` object during a restart, it can check that all required data are present and provide a meaningful error message to users if anything is missing.

To test the capability, a single-channel, single-pin model was constructed with a linear ramp applied to the total power from 50 to 200% over a 2 s transient. A restart dump was made at 1 s, and the case was run to completion. A second case was run, restarting from the 1 s point in the transient that was generated by the first case. Edits were made from each of the two cases every 0.5 s, meaning the first case had five edit groups in its output file and the second had three edit groups. The correct number of edit groups were ensured to be present, and the solution data in consistent edit groups were ensured to match to within a relative tolerance of $1{\cdot}10^{-4}$. That is, groups 3, 4, and 5 of the full transient case were compared with groups 1, 2, and 3 of the restart case. This case was added as an automated regression test in CTF, which includes the comparison of edit groups.

An additional set of tests was added for the coupling interface restart procedures. For both tests, a parallel, five-assembly, quarter symmetry (three actual solved assemblies) transient model is used. The power is linearly increased from 50 to 200% over a 2 s transient. The steps in the tests are as follows.

- Run the model with CTF to 1 s.
- Save the restart data.
- Run CTF for the remainder of the transient.
- Start a new CTF simulation but initialize it from the saved restart data.
- Run the second simulation to completion.
- Compare the output files from the restarted case and the full transient case and ensure they are the same to within tolerance.

In one test, the save/load of restart data was done by using the in-memory coupling procedures, and in the other test, the save/load of restart data was done by using the procedures that direct CTF to save and load restart data. Both tests were entirely controlled via the CTF coupling interface. These tests demonstrate that all new CTF coupling interface procedures function properly for parallel CTF models.

4 MAIN STEAM LINE BREAK TRANSIENT

4.1 MODEL DESCRIPTION

The CTF systems code coupling improvements described in Section 2 were applied to realistic PWR steady-state and transient MSLB simulations of a Westinghouse 4-loop PWR.

The CTF model used in this study was a full-core nodal fidelity (2×2 radial channels per assembly) model, which was based on CASL Progression Problem 7 (Godfrey [2012]). The core specifications are based on the Watts Bar Nuclear Plant Unit 1. The nodal model uses the same 49 node axial discretization as in the pin-resolved Michigan Parallel Characteristics Transport Code (MPACT) and CTF models for Progression Problem 7, and the pin-resolved power distribution from the pin-resolved case was collapsed onto the nodal mesh to define the 3D power distribution in the nodal model.

The TRACE model is a full primary loop model of the Zion Nuclear Power Plant, which is a similar Westinghouse 4-loop design as the Watts Bar Nuclear Plant. This model was adapted from an earlier RELAP5 model of the Zion plant. Versions of the RELAP5 and TRACE models were used in the Best-Estimate Methods–Uncertainty and Sensitivity Evaluation large-break loss-of-coolant accident uncertainty project (NEA [2008]) and elsewhere (Capps et al. [2021], Barber et al. [1999]). The model is included in the TRACE V5.0 Patch 5 code distribution package provided by the NRC in which it is referred to as the "Typical PWR" model (`typPWR.inp`). The specific version of the model used for the present work is the one provided within the Symbolic Nuclear Analysis Package (SNAP) distribution (Applied Programming Technology [2021]) exported to TRACE via SNAP version 3.1.5.

A diagram of the TRACE model is given in Figure 3. The four physical primary loops are grouped into two solved loops in the model: a "broken loop" to which a main steam line or cold leg break may be applied and the remaining three "intact loops" lumped into one combined loop. The pressurizer (attached to the intact loop), steam generators, accumulators, reactor coolant pump (RCP), and vessel are explicitly modeled. Relief valves, isolation valves, charging flow, and reactor scram are modeled by using appropriate set point-based trips.

A valve component attached to the broken loop steam line was included in the model to simulate an MSLB. The valve flow area in the fully open position was originally set to 0.0873 ft^2, which is equivalent to a 4 in. diameter break. This small break size led to a much slower transient than was desired for this demonstration, giving a gradual depressurization of the primary system over several minutes of transient time. To provide a transient that was a more challenging demonstration of the CTF-TRACE coupling, testing the ability to react to more rapid T/H changes, the break size was increased to 2.65 ft^2 (22 in. effective diameter). This is the break size that was specified for the Organisation for Economic Co-operation and Development PWR MSLB benchmark (Ivanov et al. [1999]), which is used to represent a full double-guillotine break of the main steam line. This 22 in. diameter break was assumed for the present study, and it led to reasonable consistency with the published benchmark results (Beam et al. [2000]) in terms of depressurization rate, scram time, core inlet temperature response, and other relevant parameters.

As noted in Section 2, the current CTF-TRACE coupling does not support the exchange of radially dependent core T/H BCs. Only full-core BC values can be currently exchanged. For this reason, the core in the TRACE MSLB model was represented as a single channel, which is consistent with the original `typPWR.inp` model. In reality, a break in a single steam line with the remaining three loops intact would

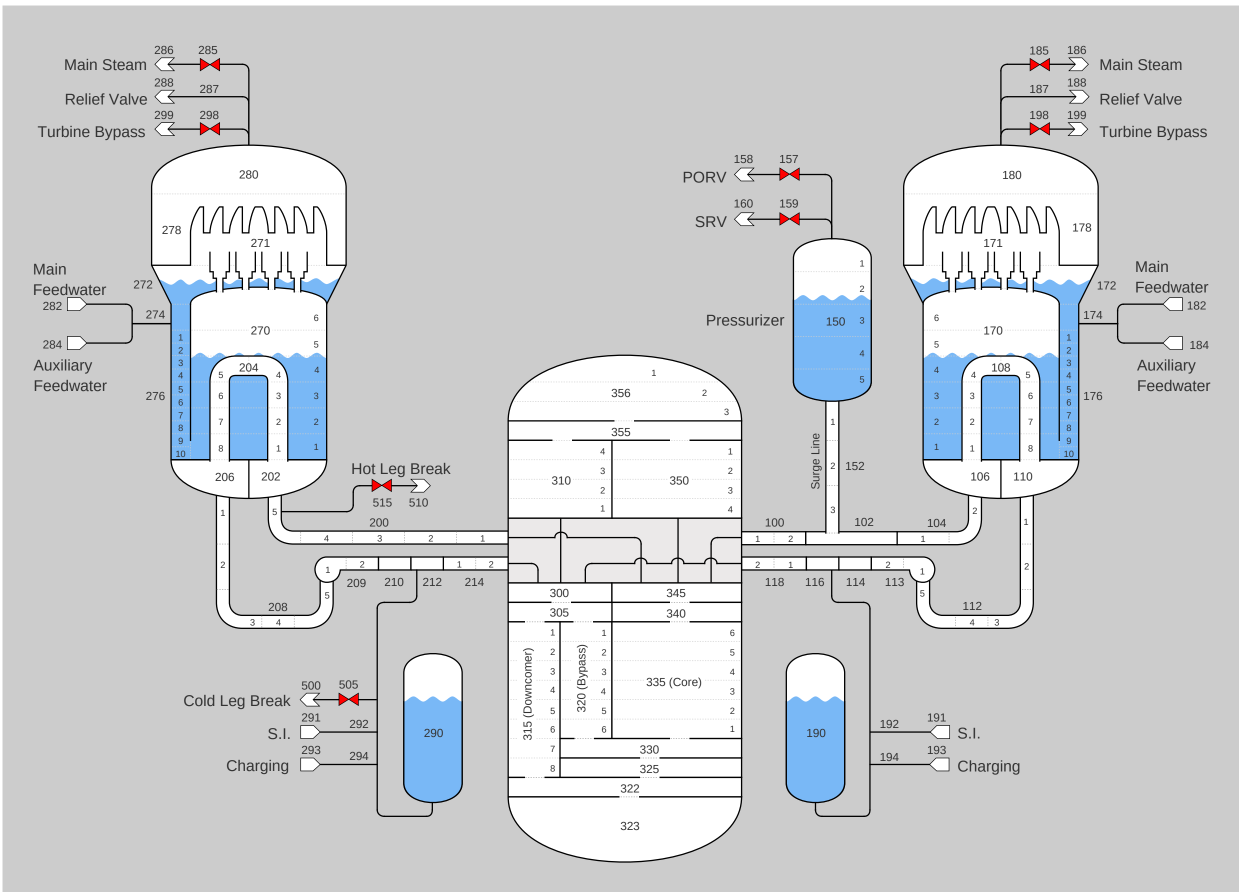


Figure 3. Diagram of the TRACE model used for the MSLB simulation (Applied Programming Technology [2021]).

lead to significant asymmetry in the core inlet temperature and flow distributions. This behavior is not represented in the current demonstration, but future work will implement finer radial discretization in the TRACE model and add the necessary coding changes in CTF to support radially dependent BCs in the coupling.

The current TRACE model uses point kinetics with no T/H reactivity feedback; only scram reactivity is modeled. Therefore, the current TRACE model does not exhibit an initial power increase (MSLB benchmark results in a roughly 20% predicted increase in core power before scram) nor does it account for the possible recriticality and return to power that was predicted by some of the point kinetics codes in the benchmark study within approximately 60 s following scram. However, the focus of the present work is to demonstrate T/H coupling between CTF and TRACE, and accurate neutronic feedback will be introduced subsequently by coupling with MPACT.

4.2 RESULTS

The MSLB transient was performed with coupled CTF-TRACE by using the overlapping domain approach. Results are presented in this section for both the one-way (TRACE to CTF) and two-way coupling schemes described in Section 2

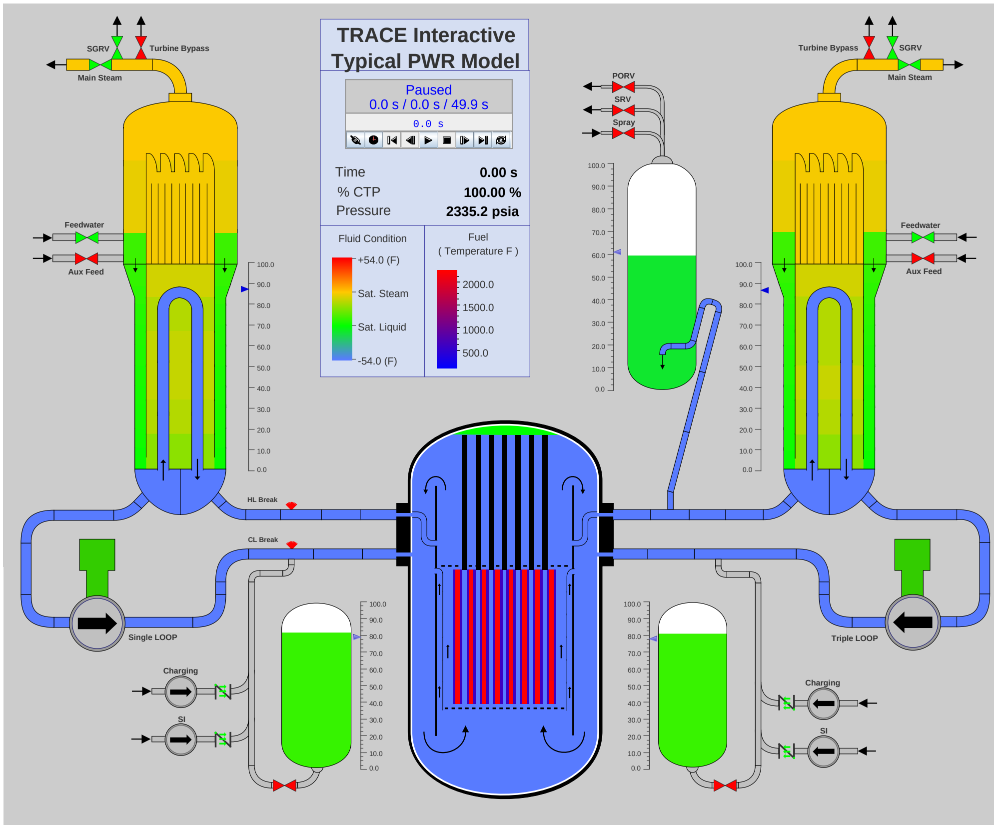
The transient progression is shown in Figures 4–8 at five different time points during the simulation. These results were obtained for the two-way coupling; however, the overall transient progression for the one-way coupling was similar.

The 22 in. diameter rupture of one of four steam lines is applied at t = 1.0 s. Closure of the main steam isolation valve (MSIV), safety injection, charging flow, and reactor scram are initiated automatically based on the pressure setpoints and response times included in the model.

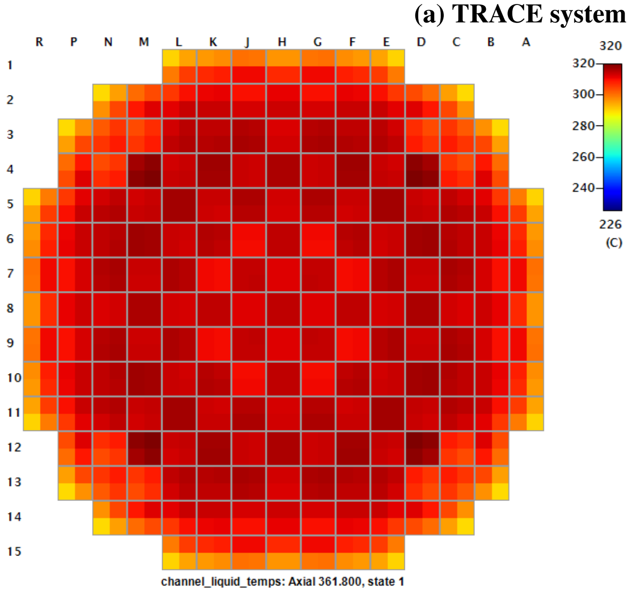
Currently, no reactor power information (i.e., scram time, reactivity, or core power) is passed from TRACE to CTF. In future work, the ECI will be used to provide TRACE-predicted scram time or scram reactivity to MPACT, and the resulting core power distribution will be applied to CTF and possibly also to TRACE through the ECI. In the present work, a simplified approach was used in which the time-dependent core power calculated by TRACE was determined from a stand-alone TRACE simulation of the MSLB event, and this was applied to CTF as a power-forcing function in the CTF input file. Recall that T/H reactivity feedback is not enabled in the current TRACE model; therefore, calculating the core power vs. time in the absence of CTF coupling is acceptable for the purposes of this study.

Figures 9–11 show the time-dependent core inlet temperature, core inlet flow rate, and core outlet pressure BC values in CTF compared with the values provided in the TRACE output plot file. The TRACE and CTF results are in full agreement at every time step throughout the transient; the apparent difference, particularly in the first 5 s, is only because the TRACE results are shown at every 0.1 s vs. the CTF results that are shown at every time step. This perfect agreement between the codes verifies that the correct values were transferred through the ECI and successfully applied to CTF. These values are shown for the two-way coupling case; the same successful verification of boundary values for the one-way coupling case was also performed.

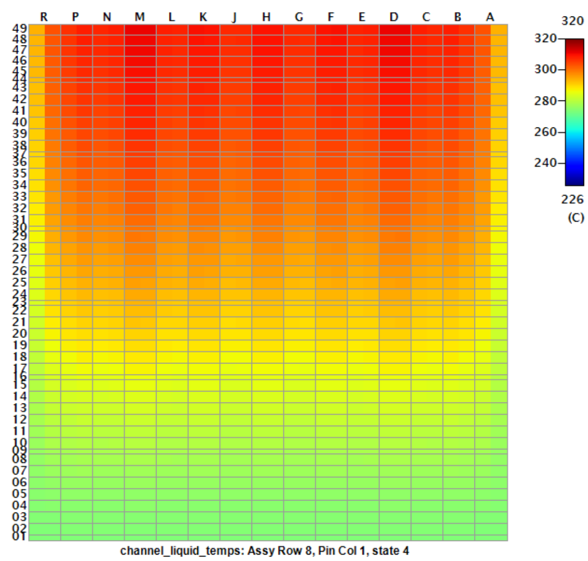
The one-way and two-way coupling results are compared in Figures 12–14. TRACE predicted a lower core pressure drop than CTF (e.g., 101 kPa vs. 121 kPa at normal operating conditions). This difference is not unexpected given that the TRACE core model potentially represents a different core loading than CTF and



(a) TRACE system coolant conditions.

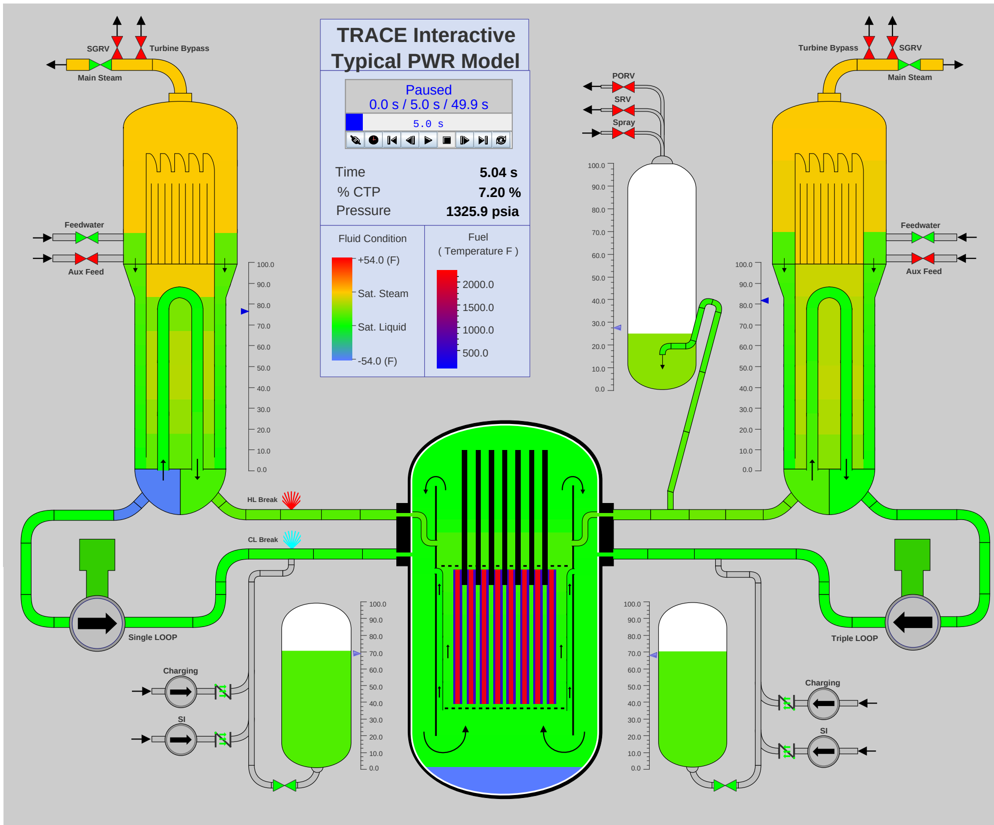


(b) CTF coolant outlet temperature (top-down view).

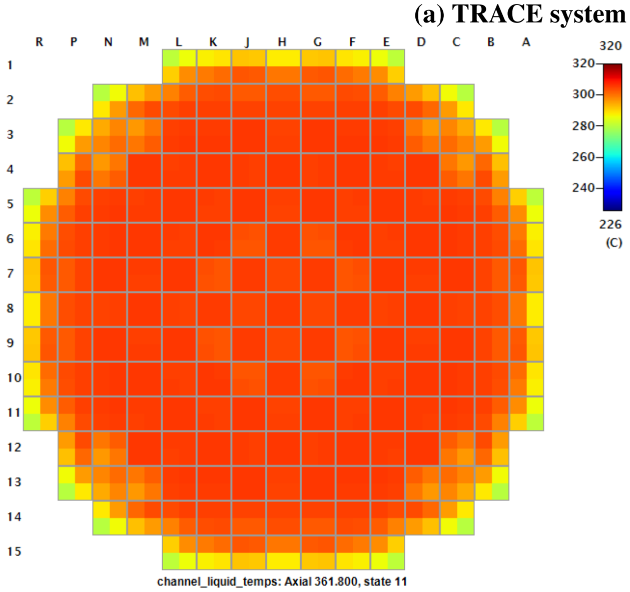


(c) CTF coolant temperature (side view).

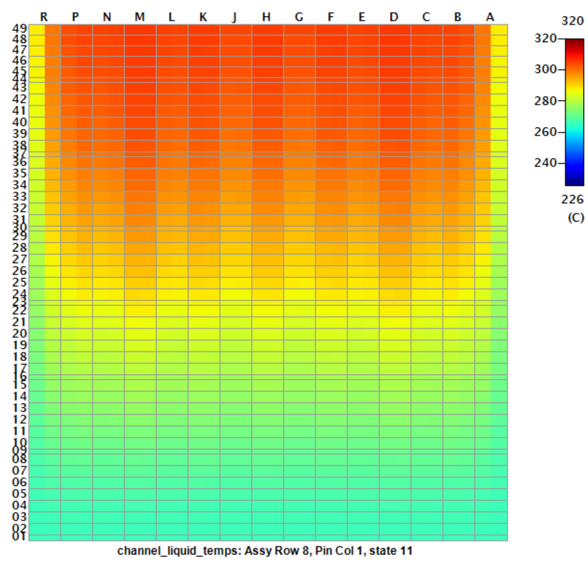
Figure 4. MSLB results at t = 0 s.



(a) TRACE system coolant conditions.

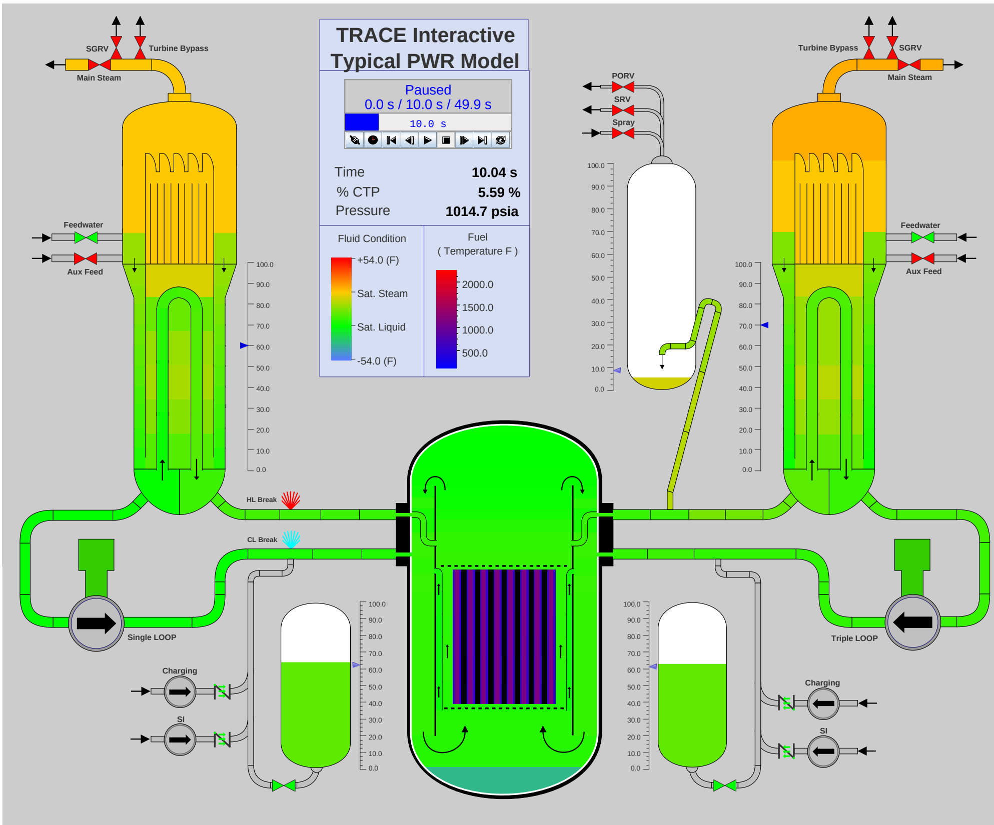


(b) CTF coolant outlet temperature (top-down view).

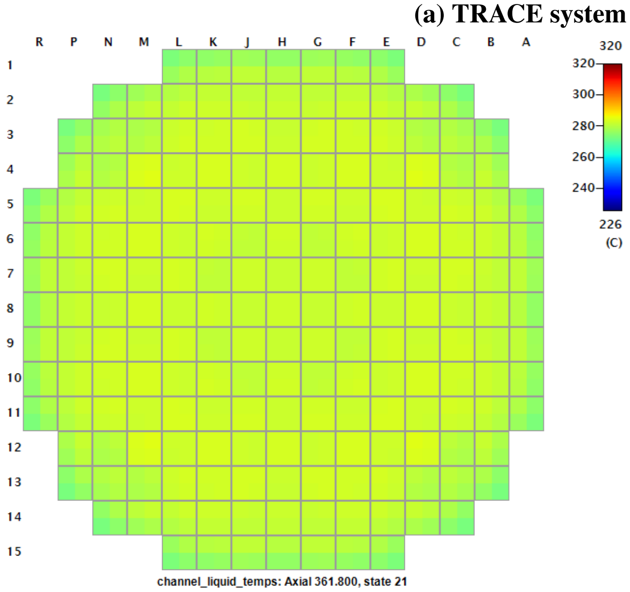


(c) CTF coolant temperature (side view).

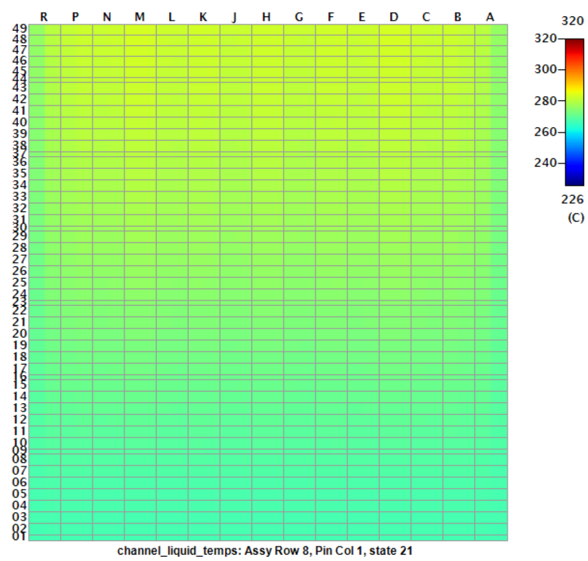
Figure 5. MSLB results at t = 5 s.



(a) TRACE system coolant conditions.

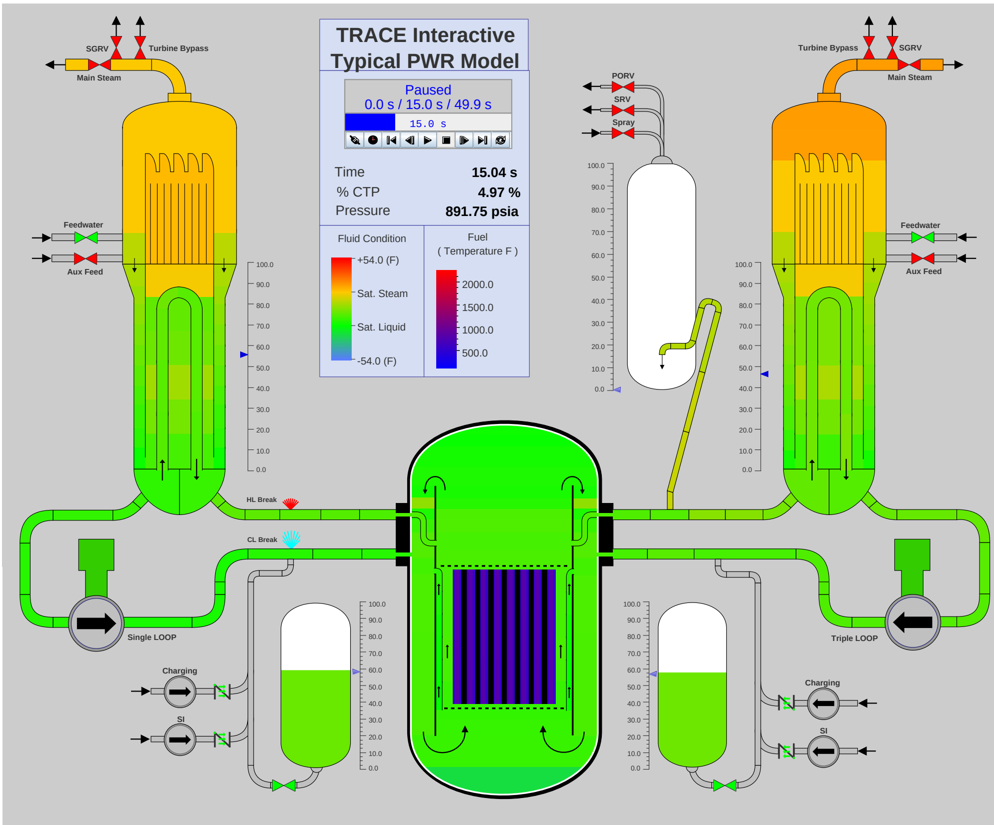


(b) CTF coolant outlet temperature (top-down view).

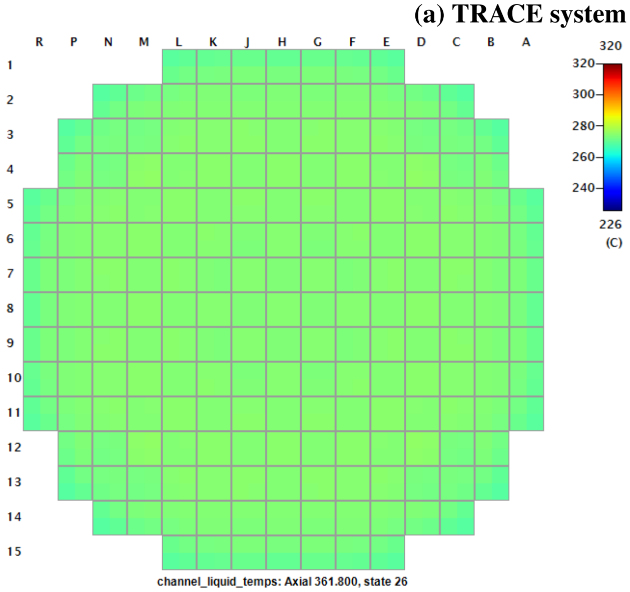


(c) CTF coolant temperature (side view).

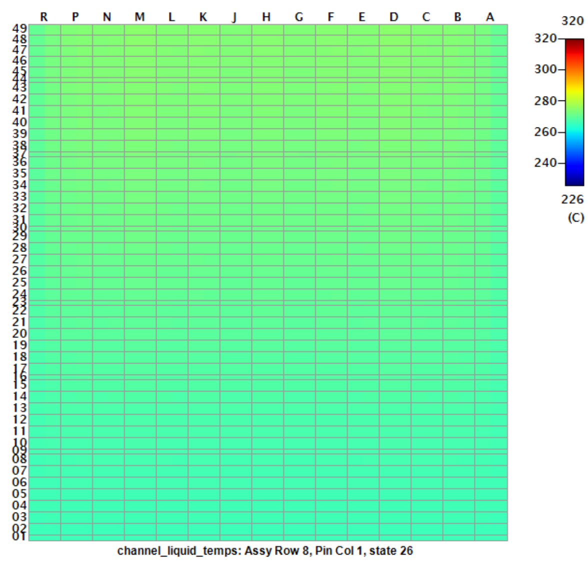
Figure 6. MSLB results at t = 10 s.



(a) TRACE system coolant conditions.

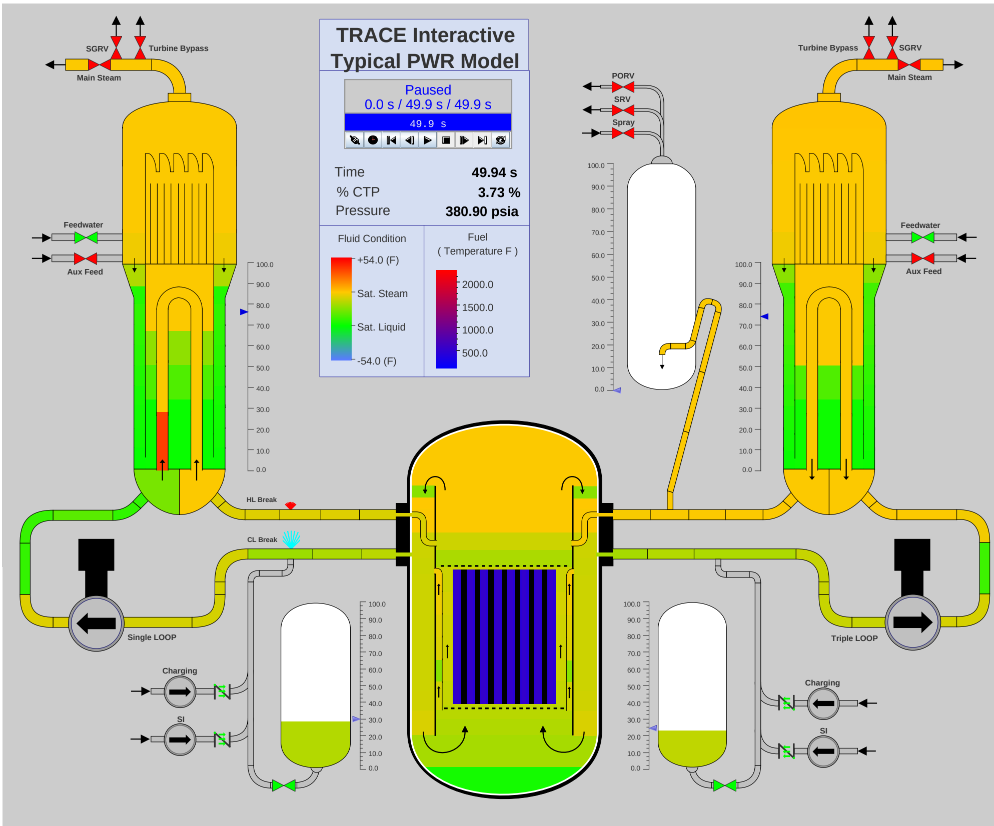


(b) CTF coolant outlet temperature (top-down view).

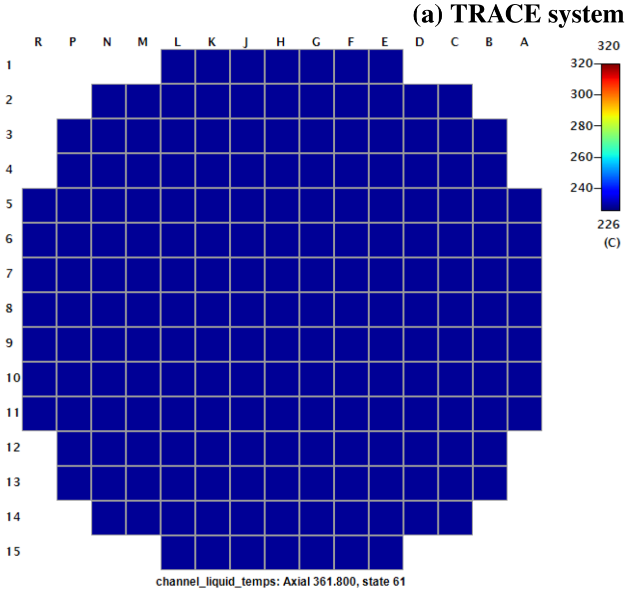


(c) CTF coolant temperature (side view).

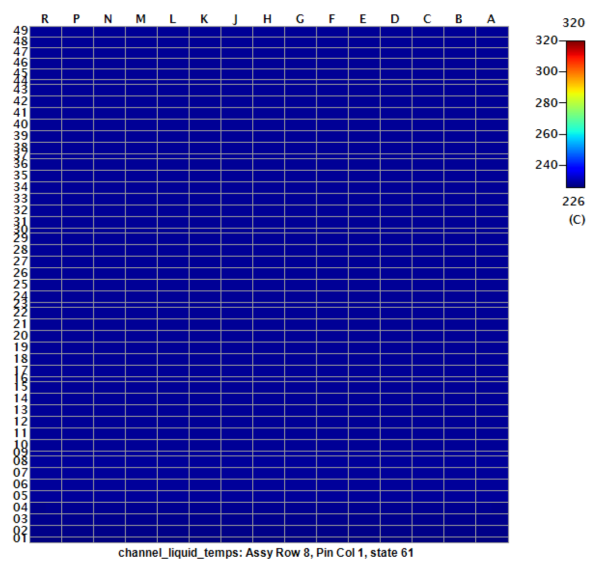
Figure 7. MSLB results at t = 15 s.



(a) TRACE system coolant conditions.



(b) CTF coolant outlet temperature (top-down view).



(c) CTF coolant temperature (side view).

Figure 8. MSLB results at t = 50 s.

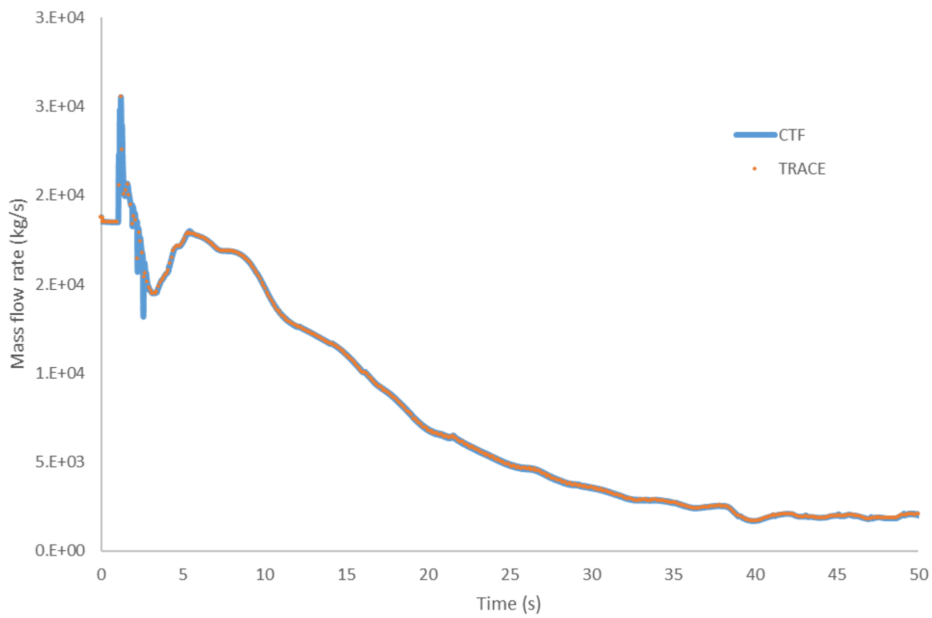


Figure 9. Core inlet flow rate reported by CTF and TRACE during the MSLB event.

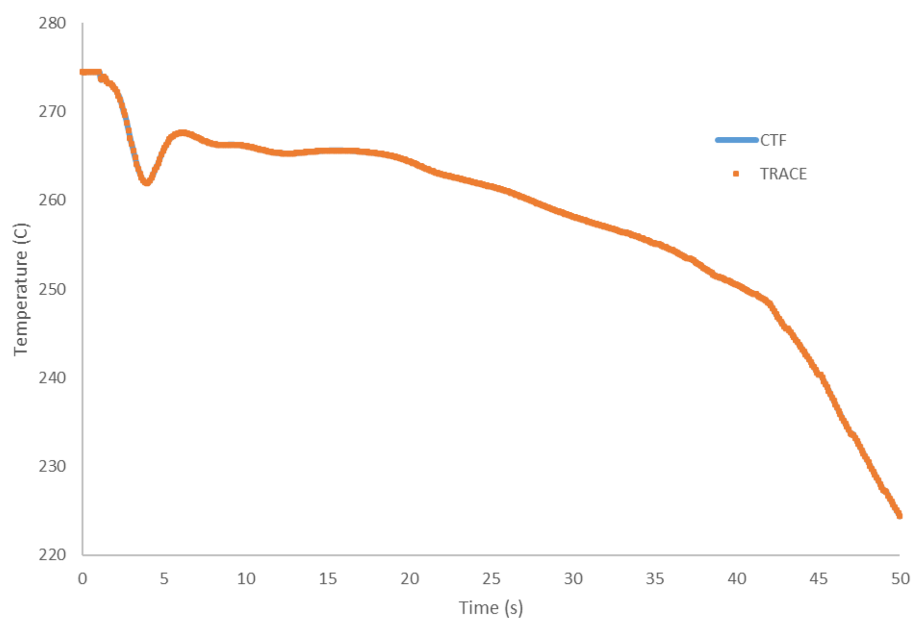


Figure 10. Core inlet temperature reported by CTF and TRACE during the MSLB event.

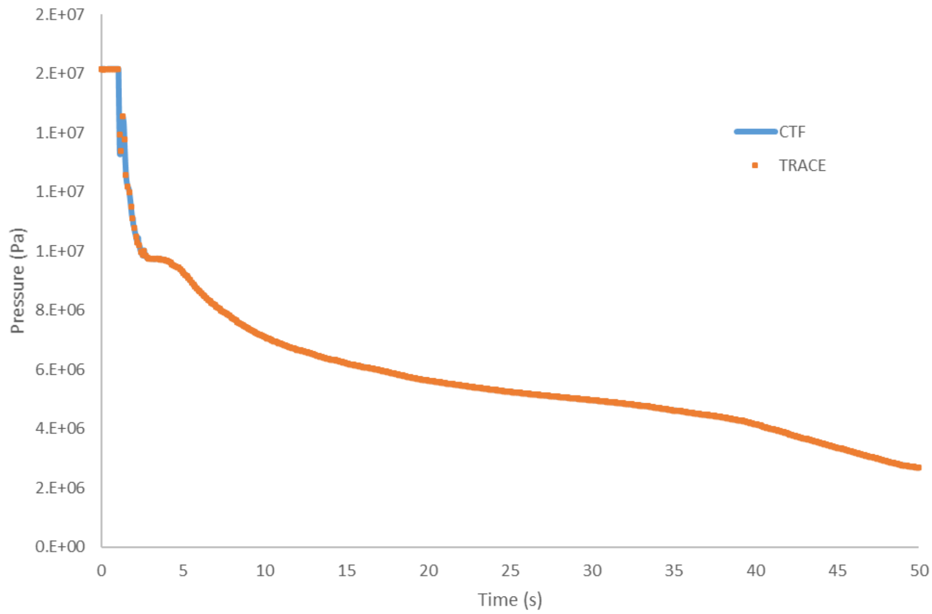


Figure 11. Core outlet pressure reported by CTF and TRACE during the MSLB event.

uses a much coarser nodalization (one radial node for the whole core vs. 2×2 radial nodes per assembly). The CTF pressure drop feedback applied to TRACE resulted in an approximately 1.6% lower primary loop flow rate at normal operating conditions and a slightly reduced flow rate for most of the transient compared with the one-way feedback case. The unadjusted TRACE model predicts that 17% of the total primary loop pressure loss is contributed by the core (101 kPa core pressure drop vs. 556 kPa RCP head). The roughly 9% core pressure drop correction (20 kPa at normal operating conditions) applied by the CTF feedback equates to approximately 1.57% correction in total loop pressure drop. The RCP rotational speed was held at a fixed 124.5 rad/s in both cases, and the impact of the loop pressure drop on the loop flow rate is determined by the built-in Westinghouse RCP performance curves; however, a 1.6% flow rate change due to the 1.6% pressure drop change is reasonable.

A few sharp spikes are observed in the calculated mass flow rates between $t = 1$ and $t = 5$ s. Such spikes are seen even in the one-way coupling case in which the CTF-calculated solution does not impact the TRACE solution. This indicates that the spikes are a result of the TRACE calculation and are not indicative of instability in the two-way coupling. These spikes could be the result of physical processes (e.g., valve closures) within the TRACE model and/or could be a temporary numerical artifact in the system calculation. This behavior is often seen for system T/H codes; for example, similar spikes can be found in the published results for the MSLB benchmark problem across multiple different systems codes (Beam et al. [2000]). Importantly, including CTF feedback in the TRACE solution did not appear to reduce the stability of the TRACE solution.

The time step sizes during the MSLB event are shown in Figure 15. The `SystemCoupling_type` enforces the same time step size in both codes based on both codes' CFL-based time step limits and the maximum allowable time step sizes (`dtmax`) set in the codes' input files. In this case, a `dtmax` of 0.001 s was set in both codes, and this was the actual time step size used for most of the calculation, except at certain points when the numerics required a temporary time step size reduction. The fact that the time step size reached

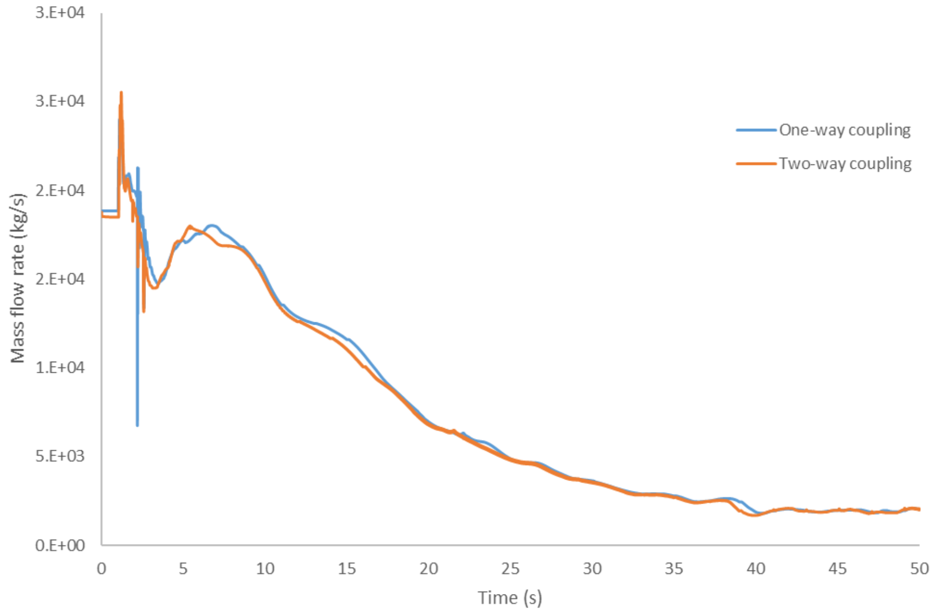


Figure 12. Core inlet mass flow rate during the MSLB event.

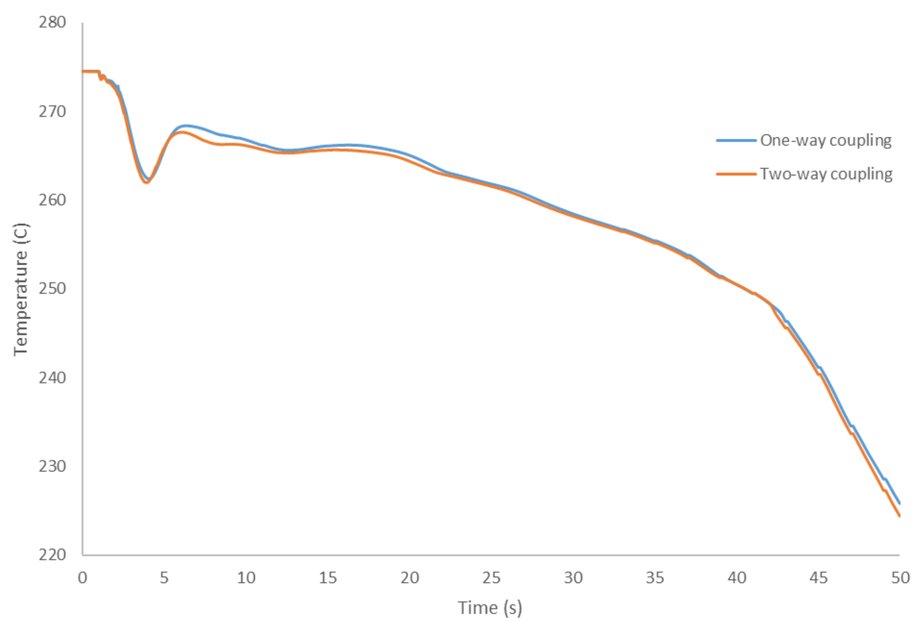


Figure 13. Core inlet temperature during the MSLB event.

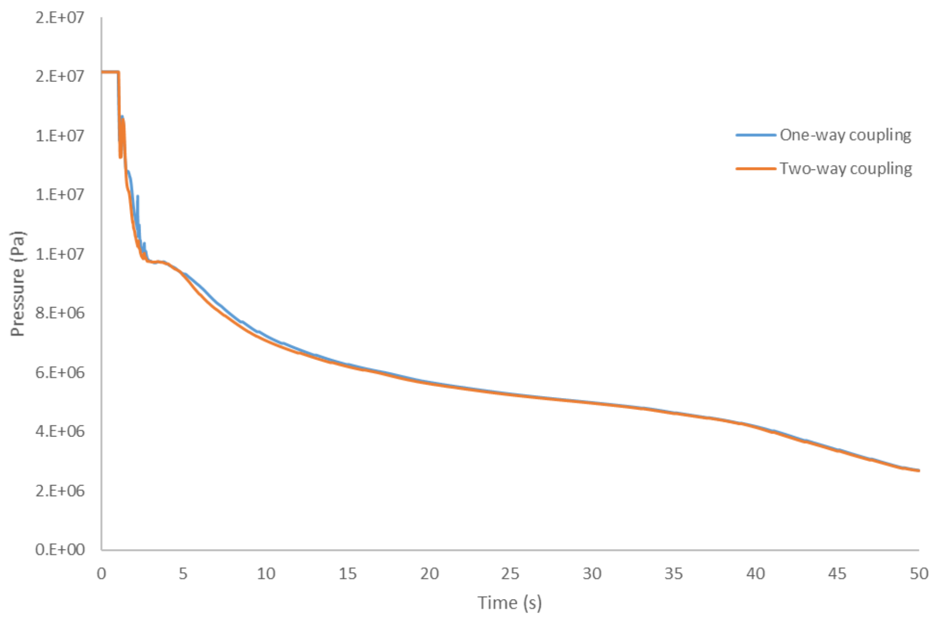


Figure 14. Core outlet pressure during the MSLB event.

`dtmax` for most of the event in both the one-way and two-way coupling cases indicates that the two-way coupling did not appreciably impact the codes' numerical stability for this problem.

Importantly, in the previous coupling work (Wysocki et al. [2019]), the inherent numerical instability of the nonoverlapping domain coupling approach led to time step sizes on the order of $1{\cdot}10^{-5}$ s throughout each transient simulation, even for null or mild transients. The fact that the overlapping domain approach produced $1{\cdot}10^{-3}$ s time step sizes—which could have been even higher if a larger `dtmax` were used—demonstrates the superior numerical stability of the overlapping domain approach relative to the previous nonoverlapping domain scheme.

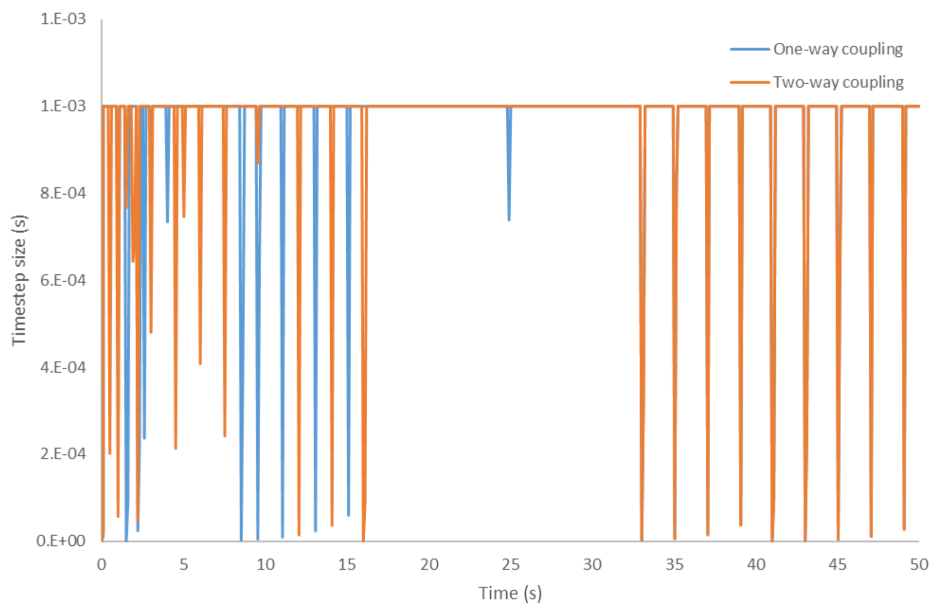


Figure 15. CTF and TRACE time step size during the MSLB event.

5 SUMMARY

Significant improvements were made to the CTF system code coupling capabilities, including the implementation of an overlapping domain coupling approach and the initial implementation of pressure drop feedback in which a correction is applied to ensure that the TRACE core pressure drop better matches the CTF core pressure drop. The resulting coupling is more numerically robust and allows larger time step sizes than the explicit nonoverlapping domain coupling implemented previously.

A more flexible input specification was implemented that allows users to define nonoverlapping or overlapping domain coupling with one- or two-way feedback, depending on which physical quantities users specify for transfer and the location within the TRACE model at which the transfers will occur. Support for coupling parallel CTF models to serial TRACE models was added. A restart capability was also implemented into CTF, which will be used in the future for restarting CTF-TRACE simulations at specific points in the transient simulation.

Future effort will focus on the following tasks.

- Add MPACT to the CTF-TRACE coupling to provide an accurate 3D core power response during coupled transients
- Fully implement a coupled restart capability, which will be used to restart or resume a transient calculation from a specified point in the simulation. This will require the further development of CTF and MPACT restart capabilities, as well as driving a TRACE restart calculation from the requested restart point.
- Achieve the ability to exchange radially dependent core T/H BC data between CTF and TRACE, allowing for the accurate modeling of asymmetric T/H conditions during transients.
- Improve the pressure drop correction capability, including a more advanced relaxation factor implementation for optimized performance.
- Achieve the ability to specify additional coupling options in the input file, including steady-state coupled convergence tolerances.

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