IMPLICIT TIME-INTEGRATION METHOD
FOR SIMULTANEOUS SOLUTION OF A
COUPLED NON-LINEAR SYSTEM

A Dissertation in
Nuclear Engineering
by
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Abstract

Historically large physical problems have been divided into smaller problems based on the physics involved. This is no different in reactor safety analysis. The problem of analyzing a nuclear reactor for design basis accidents is performed by a handful of computer codes each solving a portion of the problem. The reactor thermal hydraulic response to an event is determined using a system code like TRAC RELAP Advanced Computational Engine (TRACE). The core power response to the same accident scenario is determined using a core physics code like Purdue Advanced Core Simulator (PARCS). Containment response to the reactor depressurization in a Loss Of Coolant Accident (LOCA) type event is calculated by a separate code. Sub-channel analysis is performed with yet another computer code. This is just a sample of the computer codes used to solve the overall problems of nuclear reactor design basis accidents. Traditionally each of these codes operates independently from each other using only the global results from one calculation as boundary conditions to another. Industry’s drive to uprate power for reactors has motivated analysts to move from a conservative approach to design basis accident towards a best estimate method. To achieve a best estimate calculation efforts have been aimed at coupling the individual physics models to improve the accuracy of the analysis and reduce margins. The current coupling techniques are sequential in nature. During a calculation time-step data is passed between the two codes. The individual codes solve their portion of the calculation and converge to a solution before the calculation is allowed to proceed to the next time-step. This thesis presents a fully implicit method of simultaneous solving the neutron balance equations, heat conduction equations and the constitutive fluid dynamics equations. It discusses the problems involved in coupling different physics phenomena within multi-physics codes and presents a solution to these problems. The thesis also outlines the basic concepts behind the nodal balance equations, heat transfer equations and the thermal hydraulic equations, which will be coupled to form a fully implicit nonlinear system of equations.
The coupling of separate physics models to solve a larger problem and improve accuracy and efficiency of a calculation is not a new idea, however implementing them in an implicit manner and solving the system simultaneously is. Also the application to reactor safety codes is new and has not be done with thermal hydraulics and neutronics codes on realistic applications in the past. The coupling technique described in this thesis is applicable to other similar coupled thermal hydraulic and core physics reactor safety codes. This technique is demonstrated using coupled input decks to show that the system is solved correctly and then verified by using two derivative test problems based on international benchmark problems the OECD/NRC Three mile Island (TMI) Main Steam Line Break (MSLB) problem (representative of pressurized water reactor analysis) and the OECD/NRC Peach Bottom (PB) Turbine Trip (TT) benchmark (representative of boiling water reactor analysis).
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Nomenclature

\[ \nu = \text{neutron speed} \]

\[ t = \text{time} \]

\[ \chi_p = \text{fraction of prompt fission neutrons} \]

\[ \chi_d = \text{fraction of delayed fission neutrons} \]

\[ \beta = \text{delayed-neutron fraction} \]

\[ \Sigma_f = \text{macroscopic fission cross section} \]

\[ \Sigma_{tr} = \text{macroscopic transport cross section} \]

\[ \Sigma_R = \text{macroscopic scattering cross section} \]

\[ \Sigma_{sg \rightarrow g} = \text{macroscopic scattering cross section from group } g \text{ to } g' \]

\[ \Sigma_a = \text{macroscopic absorption cross section} \]

\[ \lambda = \text{decay constant} \]

\[ \phi = \text{neutron flux} \]

\[ J = \text{neutron current} \]

\[ C_I = \text{precursor density} \]

\[ V = \text{volume} \]

\[ D = \text{diffusion coefficient} \]

\[ \alpha = \text{gas volume fraction} \]

\[ \rho_l = \text{liquid phase density} \]

\[ \rho_g = \text{gas phase density} \]

\[ V_l = \text{liquid phase velocity} \]

\[ V_g = \text{gas phase velocity} \]

\[ P = \text{total pressure} \]

\[ f_l = \text{liquid vapor interfacial friction} \]
\( f_{wg} \) = wall drag for gas phase
\( f_{wl} \) = wall drag for liquid phase
\( \Gamma \) = interfacial mass-transfer rate
\( e_g \) = gas phase internal energy
\( e_l \) = liquid phase internal energy
\( q_{wg} \) = heat-transfer rate per unit volume to the gas phase
\( q_{wl} \) = heat-transfer rate per unit volume to the liquid phase
\( q_{dg} \) = power deposited directly to the gas phase
\( q_{dl} \) = power deposited directly to the liquid phase
\( C_i \) = friction coefficient for the interface between gas and liquid
\( C_{wg} \) = friction coefficient between the wall and gas phase
\( C_{wl} \) = friction coefficient between the wall and liquid phase
\( C_p \) = specific heat
\( k \) = thermal conductivity
\( q'' \) = heat generation rate per unit volume
\( q_{total} \) = total heat flux
\( h_l \) = convective HTC for the liquid phase
\( h_g \) = convective HTC for the gas phase
\( T_w \) = temperature of the wall
\( T_l \) = temperature of the liquid phase
\( T_g \) = temperature of the gas phase
\( C_B \) = soluble boron concentration
Chapter 1

INTRODUCTION TO COUPLED NUCLEAR REACTOR SAFETY ANALYSIS

The purpose of this document is to present an innovative way to resolve the deficiencies in the current state-of-the-art coupled thermal hydraulics and neutronics codes that are known to exist. The implementation of this solution will greatly improve the accuracy of the analysis capabilities for light water nuclear reactors.

This chapter will introduce the concepts necessary to develop the coupled reactor safety code system. This introduction will discuss the previous and current state-of-the-art methods for coupling code systems simulating different physics phenomena and their application to the field of nuclear engineering. This chapter will also help the reader to understand the limitations of the current methods and show the motivation behind this thesis. It will contain several brief sections each designed to build on the next so the reader understands the basic concepts first. It concentrates on two aspects of reactor safety the thermal hydraulic and core physics and the coupling between them. These areas are the main focus of this thesis. The first of these sections will give the reader a brief description of nuclear reactor safety analysis and design basis accidents as well as the importance of this analysis to the nuclear industry. The next several sections will discuss the solution methods used in neutronics and thermal-hydraulics as well as the current methods for coupling these two fields. In these sections an example is developed to help the reader understand the basic theory behind time integration techniques. The following chapters describe in detail the techniques used to couple the system of equations, solution methods implemented to solve the system and the verification of the model.
1.1 Nuclear Reactor Safety Analysis

In the United States of America (USA) the nuclear reactor power plants are composed of two different types of Light Water Reactors (LWR’s); Pressurized Water Reactor (PWR) and Boiling Water Reactor (BWR). A light water reactor uses common water (H$_2$O) as both the coolant and as the neutron moderation material. The water is heated using the energy released from fissioning of heavy metals such as Uranium (235U) and Plutonium (239Pu). The fission source is formed into small cylindrical pellets, which are stacked inside a tube called a fuel rod. The fuel rod has a dual purpose, it keeps the fuel in an organized configuration and it acts as a first barrier for containment of radioactive material. A fuel rod is typically half an inch in diameter and twelve foot tall. Fuel rods are grouped into a square lattice called a fuel rod bundle or a fuel assembly. The number of fuel rods in a bundle can be different based on the design and type of reactor however, a typical bundle for a PWR has between 15x15 to 17x17 fuel rods in it. A nuclear reactor core is comprised of more than a hundred fuel rod bundles. The heat generated by the fissioning of the heavy metal is removed from the fuel rods by the water. With the absorption of heat from the fuel rods the water is converted to steam. The energy stored in the steam is released by passing it through a turbine. A turbine is a large shaft surrounded by thousands of impeller blades. As the steam passing through the blades causes the shaft to turn. This shaft is connected to a generator which in turn produces electricity. This process is not unique to LWR’s. Coal and Natural gas power plant operate in a similar manor. The unique part of a nuclear power plant is the heat source. An with that unique heat source comes a world of unique problems and dangers.

The fissioning of heavy metals like 235U or 239Pu happens when an atom captures a neutron with a particular energy, the atom becomes unstable and the nucleus splits into lighter constitutive parts called fission products. In a nuclear reaction Newtonian physics no longer applies and mass is not conserved. This means that the mass of the fission products does not equal the mass of the atom before the fission process. The difference in the mass before and after the fission process is the amount of energy released during the reac-
tion. The type of fission product produced is dependent on the energy of the incident neutron. Some fission products are stable atoms while others are unstable and decay over time. Some neutrons are produced during the initial atom fission these are called prompt neutrons. Any neutrons produced through the decay of a fission process is called a delayed neutron. Initially when a neutron is produced, either prompt or delayed, it has a large amount of energy and is traveling at very high speeds. For a typical LWR the energy range for a neutron to cause another fission is below 1 eV. The neutron undergoes a process of slowing down called moderation in which the neutron energy is reduced to levels appropriate for causing another fission. The neutron looses energy by colliding with the hydrogen atom in a water molecule. Neutrons can also be absorbed by other materials in a nuclear reactor. Some of these materials are designed to absorb neutrons, like boron or control rods, and are used to help control the number of neutrons in the core at any given time. Some neutrons travel on a trajectory that leads them outside of the core where they have no probability of causing a fission, this is called neutron core leakage. It has been shown here that several neutrons are produced from one fission process and those neutrons can go on to produce another fission, leave the system, or be absorbed by another material. In order to maintain a nuclear chain reaction a balance of neutrons produced by fission and those being removed from the system must be maintained. That is the number of neutrons produced in the current generation should equal the number of neutrons produced in the previous generation. When this condition is met the nuclear chain reaction is said to be critical. If the number of neutrons in the current generation is fewer than that of the previous generation the reactor is said to be subcritical. If the number of neutrons is greater from one generation to the next the reactor is supercritical. The magnitude of the power generated by a reactor is directly proportional to the number of fissions. At this point the reader should understand that controlling the neutron population is of utmost importance in the operation of a nuclear reactor. In the case of LWR’s the neutron moderation is done with H₂O, which indicates that the neutron’s ability to slow down depends on the physical properties of water. For example, as the density of water decreases the distance between water molecules thus decreasing the probability that a neutron will collide with a hydrogen atom. The neutron behavior is dependent on many different parameters in addition to the density of water such as the boron concentration, and fuel temperature.
To accurately predict the power in a reactor core it is important to know the thermal hydraulic state of a reactor at any given time.

In the United States (US) there are two primary types of LWR’s, Pressurized Water Reactors (PWR) and Boiling Water Reactors (BWR). A pressurized water reactor is separated into two separate systems, a primary system and a secondary system. The primary system consists of a pressure vessel and several recirculation loops. The reactor core resides in the pressure vessel where the water is heated under high pressures, approximately 2000 psia. At this pressure the water does not boil but becomes very hot. This hot water is pumped to large heat exchangers called steam generators. The hot water is pumped through thousands of small tubes. The outside of these tubes are surrounded by more water, which is allowed to boil. This is called the secondary side of the reactor. From here the steam travels to the turbines. After the water in the primary side is pumped through the steam generators it is sent back to the pressure vessel and is reheated. Since the water in the primary system is constantly reused this is called a closed loop. A BWR operates in an open loop system. The water is pumped through the core and is allowed to boil. The steam produced is separated and dried in the reactor vessel. This steam is then sent to the turbines. In a BWR the fuel rod bundles are surrounded by a shroud so that the water entering the fuel rod bundle is heated within that bundle and does not mix with the rest of the core. This promotes better boiling in the core. Even though the operation of these two types of reactors is different the fundamental concepts are the same. They both use H₂O to moderate neutrons and cool the fuel rods. The cooling of the fuel rods in both reactors is paramount in the safe operation of the reactors. If allowed to get too hot the fuel rods can melt or the cladding that incases the fuel pellets could rupture allowing radio active materials to spread throughout the reactor system. In order to ensure that neither of these scenarios is possible during normal operation of a nuclear reactor redundant safety systems are designed for each reactor type. To obtain a license to operate a reactor of a particular design the reactor and safety systems are analyzed in detail to ensure, under the worst possible case, the reactor will remain in a safe configuration after a given postulated accident.
Reactor safety analysis is the determination of a nuclear reactor response to a set of postulated accident scenarios called design basis accidents. These are a set of different types of accidents divided into several different categories based on the likelihood that the accident will occur during the lifetime of a nuclear reactor. These design basis accidents are analyzed using detailed computer models. It is impossible at this time to accurately predict all of the physics and the interactions of all of the systems in a nuclear reactor. There exists some amount of conservative estimates about the physical phenomena in the safety analysis to ensure the safe operation of a reactor. In doing this a safety margin is built into the analysis. This is the set of accidents that the reactor design and licensing is based on.

In most nuclear reactor accident scenarios it is important to know the current thermal hydraulic state of the reactor (i.e. the cooling capacity) and the reactor power response to the accident. Traditionally these two systems have been analyzed using two different computer codes, one for the thermal hydraulic system and one for the core. Historically the coupling parameters (boron concentrations, densities, temperatures, powers, etc.) have been input into the individual codes as boundary conditions. Current state-of-the-art methods pass these coupling parameters between the computer codes using libraries designed to run two separate computer codes at once and pass information between them such as Parallel Virtual Machine (PVM), or the codes have been integrated to the point of producing one executable image but retaining the separate solvers, input, output, and processing. In either case the time integration is very important to determine the calculational time step size. Several different time integration techniques have been developed which are used in the nuclear industry for solving time dependent problems on computers. The techniques are explicit, semi-implicit, Stability Enhancing Two-Step (SETS), and implicit methods. These methods will be discussed further in later sections of this chapter.

The discussion up to this point should have a sufficient amount of detail for the reader to understand the complexity of a nuclear reactor and the importance reactor safety analysis plays in the safe operation of a nuclear reactor.
1.2 Solution Techniques

The complexity of the physics in a nuclear reactor make it impossible to analytically solve the governing equations. Instead computers are used to make a model of the system. To do this the governing equations need to be developed into a form which can be solved numerically by a computer. In doing so approximations and assumptions are made about the equations used in the model. This is done by relating the equations to small discrete volumes, which represent the actual system in both space and time. The process of converting the differential equations to this form is called discretization. This section of the thesis summarizes some of the techniques used to formulate the discrete equations discussed in this thesis.

1.2.1 Spatial discretization

It is not possible to solve the physics problems presented in this thesis analytically. Therefore, it is necessary to approximate the problems numerically. This is done by writing the governing differential equations in finite difference form. The new formulation can then be easily solved on a computer. A finite difference is defined as the functional difference between two points in the form, \( f(x + a) - f(x + b) \). In general three different finite difference formulations are used, Forward Differencing (FD), Backward Differencing (BD), and Central Differencing (CD) shown in equations (1-1) to (1-3).

\[
\text{FD} : f'(x) = \frac{f(x + h) - f(x)}{h} \quad (1-1)
\]

\[
\text{BD} : f'(x) = \frac{f(x) - f(x - h)}{h} \quad (1-2)
\]

\[
\text{CD} : f'(x) = \frac{f\left(\frac{x + h}{2}\right) - f\left(\frac{x - h}{2}\right)}{h} \quad (1-3)
\]
If any of these differencing expressions are divided by \( h \), assuming \( h \) is very small, equation (1-4) can be used to accurately representation of the derivative of the function \( f'(x) \).

\[
f'(x) = \lim_{h \to 0} \frac{f(x + h) - f(x)}{h} \approx \frac{f(x + h) - f(x)}{h}
\]  

(1-4)

These are basis for different techniques for writing differential equations in finite difference form. There are many different ways to generate finite difference forms of differential equations. I will discuss two different schemes, which are commonly used in TRACE and PARCS. The first method is based on a taylor series expansion to approximate a function. Given some second order differential equation:

\[
\frac{d^2 \Psi}{dx^2} + \Psi(x) = 0
\]

(1-5)

To write the discrete form of equation (1-5) at cell \( i \) for the one-dimensional problem shown in Figure 1-1 we first need to approximate the second order derivative term. To simplify this example we will assume that the cell length are the same for all cells. The first step is two do a Taylor expansion for cells \( x_{i-1} \) and \( x_{i+1} \) in terms of cell \( x_i \) and neglect terms higher than the second order derivative.

\[
\Psi(x_{i-1}) = \Psi(x_i) - h \frac{d \Psi}{dx} \bigg|_i + \frac{h^2}{2} \frac{d^2 \Psi}{dx^2} \bigg|_i
\]

(1-6)

Figure 1-1 : Finite Difference Cell Indexing
If we add equations (1-6) and (1-7) together we get the central difference formulation for the second order derivative term, equation (1-8).

$$\frac{d^2\Psi}{dx^2} = \frac{\Psi(x_{i+1}) - 2\Psi(x_i) + \Psi(x_{i-1})}{h^2}$$

(1-8)

Then the final finite difference form of equation (1-5) is:

$$\frac{\Psi(x_{i+1}) - 2\Psi(x_i) + \Psi(x_{i-1})}{h^2} + \Psi(x_i) = 0$$

(1-9)

The second scheme involves integrating the original equation over a generic cell length. The integrals are then approximated using averaged properties and differencing techniques. The details of this method will not be presented here since they rely more heavily on the particular equation being solved. References [1][2] has more details on this topic.

Similar to the finite difference method TRACE and PARCS use the finite volume method. In this method the differential equations are integrated over a volume surrounding a discrete point. Using this method the divergence terms for example, in the fluid equations can be converted to surface integrals using the divergence theorem. The surface integrals are then formulated as fluxes at the surface of the volume. The fluxes leaving one finite volume are equal to the fluxes entering the adjacent finite volume. This indicates that this method is conservative. The details of this technique can be found in [3][24].

There have been several different methods used for the spatial solution of the neutron balance equation. The method proposed in this document is only utilizing the coarse mesh finite difference portion of the PARCS solution so the details of other methods will not be covered in this document. However, the reader should be aware that such methods like
fine mesh finite difference, coarse mesh, and nodal methods exist. The fine mesh or finite
element methods are used when very detailed models of the core are necessary. When a
course mesh can be used the coarse mesh finite difference and nodal methods represent
relatively large (regions larger than a diffusion length) homogeneous region of the core[4].
PARCS uses the coarse mesh finite difference method coupled with an analytic nodal
method to correct the leakage terms in the finite difference representation.

1.2.2 Time Integration Techniques

Analogous to the spatial discretization of the differential equations, the equations also
need to be discretized in time. Several different techniques have been used to represent
the changes in functions with respect to time. The most common techniques are the
explicit, semi-implicit, and implicit time integration methods. This section will summa-
rize the basic concepts behind each of these methods and is meant as an introduction to
each method so that the reader will understand the basic concepts of each method. The
application of each of these techniques to reactor analysis and the limitations of each tech-
nique will be covered in later sections.

Explicit time integration method is based on a truncated Taylor expansion and is often
referred to as a Forward Euler Method, [1][2]. We can expand some function $y(t)$ around
t = $t^n$ such that we get a truncated Taylor expansion, shown in equation (1-10).

\[
y^{n+1} = y(t^n + \delta t) = y(t^n) + \delta t \frac{dy(t^n)}{dt} + O(\delta t^2)
\]

(1-10)

The $O(\delta t^2)$ in equation (1-10) represents the Local Truncation Error (LTE) for this
method. In this example this method is first order. If we truncate the Taylor expansion at
higher orders then the LTE decreases assuming the same time step size and the time step
size resolves the physical time scale of the problem being solved. Since explicit methods
depend explicitly on know quantities they are simple to implement. However, this method
is only numerically stable for small time step sizes. In the case of fluid dynamics the maximum time step size is the sonic courant stability limit shown in equation (1-12). For time steps larger than the value computed in the stability limit the solution will diverge. Equation (1-11) shows the explicit representation of the gas mass conservation equation.

\[
\frac{\partial \alpha \rho_g}{\partial t} + \nabla \cdot (\alpha \rho_g \mathbf{V}_g) = \Gamma_i
\]

Equation (1-12) shows the courant limit. The \( k \) parameter varies depending on the method but is assumed to be 1.0 in TRACE. \( c \) is the speed of sound, \( \mathbf{V} \) is the flow velocity, and \( \Delta x \) is the cell length.

\[
\Delta t \leq k \frac{\Delta x}{|\mathbf{V}| + c}
\]  

The Implicit method or Backward Euler Method is numerically stable for all time step sizes. This is usually the desired method in applications where the stability of explicit method is very limiting on the time step size. The Taylor expansion for the Backward Euler Method is given in equation (1-13).

\[
y^n = y(t^{n+1} - \delta t) = y(t^{n+1}) - \delta t \frac{dy}{dt} + O(\delta t)^2
\]  

This method is numerically stable for all \( \delta t > 0 \), however it is harder to implement and is more computational expensive for each time step than the explicit method. Equation (1-14) show the implicit representation of the gas mass equation.

\[
\frac{\alpha^n + 1}{\Delta t} \rho_g^n + \nabla \cdot (\alpha^n \rho_g^n \mathbf{V}_g^n) = \Gamma_i^n
\]
Semi-implicit methods relax the time step size associated with the explicit method by evaluating the pressure gradient and the velocities involved in the mass and energy equations at the new-time level. Equation (1-15) shows the semi-implicit representation of the gas mass equation.

\[
\frac{\alpha^{n+1}\rho_g^n - \alpha^n\rho_g^n}{\Delta t} + \nabla \cdot (\alpha^n \rho_g^n \mathbf{v}_g^{n+1}) = \Gamma_i^{n+1}
\]  

(1-15)

With the pressures and velocities known at the same time step for all cells any pressure disturbance is also known in every cell. This means that the speed of sound can be removed from equation (1-12). The new limit is called the material stability limit and is shown in equation (1-16).

\[
\Delta t < \frac{k \Delta x}{|\mathbf{v}|}
\]

(1-16)

The paragraph above uses conservation of mass equation from TRACE as an example. However, the method used in PARCS is the theta method which is discussed in more detail in Chapter 2. Each of the methods above (explicit, implicit, and semi-implicit) can be derived from the theta method[4].

1.3 Current Methods of Coupling Multi-Physics Codes

Initially reactor safety analysis consisted of the use of detailed physics codes that focused on a specific aspect of the analysis and included crude models for other systems. For instance, thermal hydraulics codes such as TRAC-PF1, TRAC-BF1, and RELAP5 [5][6][7] possessed the ability to accurately predict two-phase fluid flow in a reactor system. These codes generally used the reactor power as a boundary condition for the model or a point kinetics (PK) model to predict the reactor power response. On the other hand, fuel management utilized detailed three-dimensional reactor physics codes to predict the depletion of the fuel. These models usually included a very basic one-dimensional thermal hydraulics model. As computational power grew more and more efforts were placed
on improving the accuracy of the analysis. This was done by improving the simplified models used in conjunction with the detailed analysis through the coupling the detailed physics codes.

When making decisions about how to couple codes and what types of coupling is available one has to understand what is meant and what is involved in the coupling. There are two aspects to coupling different physics codes. One is the spatial coupling and the other is the temporal coupling. In the first case one has to determine how the two different codes will pass data on a spatial level. This can be an internal or external type of coupling. The second aspect looks at what point during a time step is the data spatially communicated between the two codes. Both the spatial and temporal coupling will be discussed in further detail in the following sections however, it should be pointed out at this point that the main focus of this thesis is to improve the temporal coupling of TRACE and PARCS so most of the discussion will be on that aspect of the coupling.

1.3.1 External and Internal Coupling

In general there have been two types of spatial coupling used up to this point in coupling thermal-hydraulics and neutronics codes, external and internal. External coupling is the easiest to implement and is a more basic form of coupling. Figure 1-2 shows that in this form of coupling the core physics, heat conduction, and thermal-hydraulics for the core region are calculated by one code while the remaining system is calculated using the thermal-hydraulic system code. Few parameters are passed between the two codes and are only passed at the core bottom and core top. The data passed such as pressures and mass flows are typically core average values. This method is commonly referred to as a boundary condition coupling or plenum coupling. This type of coupling was initially popular since there was very little modifications necessary to the individual code packages and computer resources for more detailed models were not available. This method however, is less accurate than more detailed models and had convergence problems caused by incon-
sistent thermal-hydraulic models in the two codes [8]. This type of coupling will not be discussed further.

As computer resources improved more detailed coupling strategies could be employed. This was done through internal coupling. The core heat transfer and thermal-hydraulic calculations were removed from the nodal code and done by the system code Figure 1-3. The core physics calculation was integrated into the system code such that one or more neutronics nodes could be coupled to a thermal-hydraulic cell, Figure 1-4. This method allows for closely coupled models in modern reactor analysis and is the method of choice for most modern code packages.
1.3.2 Spatial Coupling

With the more detailed internal coupling being used by modern reactor analysis codes one has to pay close attention to the spatial coupling of the codes. The current state-of-the-art analysis codes still maintain different spatial representations for the core physics calculations and the thermal-hydraulic calculations. It is therefore important to understand the spatial mapping of the two codes. In modern reactor analysis codes there are two mapping schemes. One method involves using a one-dimensional thermal hydraulic components to represent axial channels. Each channel is coupled to one or more neutronics node. This type of mapping is usually used for BWR cores for which there is no fluid mixing between channels. The second type of mapping maps the neutronics nodes to a thermal-hydraulic cell in a three-dimensional representation of the core or reactor vessel. Modern reactor analysis codes, such as TRACE, have two different geometrical representations for the three-dimensional components, cartesian and cylindrical. In either case, for detailed representations, both the axial and radial mappings have to be considered. Figure 1-4 shows a typical axial mapping between neutronics assemblies and a thermal-hydraulic cells. This figure shows the axial spacing for the entire core for both models, it is not common practice to vary axial representation throughout the core, except in the case of reflood calculations which are outside the scope of this dissertation. In general the neutronics representation of the core is more detailed than the thermal-hydraulics.
Figure 1-6 and Figure 1-5 show the radial coupling for the cylindrical and cartesian geometries. For typical light water reactors the core physics models are cartesian geometry, therefore the cartesian representation of the thermal-hydraulics is more convenient for a consistent coupling. Figure 1-5 shows that for cylindrical geometry the coupling is approximated.
The spatial coupling can play a role in the accuracy of results. The effects of spatial coupling on the results are not part of this thesis but are important to understand so that only the temporal coupling can be analyzed.

Figure 1-5: PWR Radial Spatial Coupling in Cartesian Geometry

Figure 1-6: PWR Radial Spatial Coupling in Cylindrical Geometry
1.3.3 Temporal Coupling

The temporal coupling and time step selection plays an important role in the coupling of reactor analysis codes. Each code has its own time-step selection algorithm based on the physics that they are trying to model. The typical approach is to use one to one time-step selection. One of codes acts as the master and the other as the slave code and both use the same time-step, which is controlled by the master. In coupled codes like TRACE/PARCS and TRAC-PF1/NEM the thermal-hydraulics code is the master time-step selector. This means that the time step selection is based on the convergence of the thermal-hydraulics parameters and global power but not the local fluxes. This has several implications to the coupled calculations. Smaller time-step sizes need to be taken to achieve accurate results. Care has to be taken to make sure the time-steps are small enough to resolve local flux distributions in fast transients with rapid power changes. Different approaches have been developed to overcome some of these deficiencies. A variable time-step control algorithm was implemented into TRAC-PF1/NEM. A meshing algorithm was developed to determine the number of neutronics time-steps that can be accomplished during a thermal-hydraulic time step based on both local neutron flux and global reactor power [9]. A similar meshing algorithm was implemented into TRAC-BF1/NEM with an additional scheme which also allowed TRAC-BF1 to advance several time-steps during one NEM time-step [8][10].

In addition to the time-step size the point at which data is exchanged between the two codes is important. These can be classified into three types of coupling, explicit, semi-implicit, and implicit schemes. Each of these schemes have their advantages and disadvantages. During one time-step, the thermal-hydraulics code computes new coolant properties: pressure, temperature, void fraction, phasic densities, boron concentration, and average fuel temperature, center line fuel temperature, and surface temperature. Some or all of these parameters are passed to the neutronics model. The neutronics model uses these parameters to update the cross sections based on the spatial mapping described above. New local fluxes are calculated and the local power is then fed back to the heat conduction model. In this description we have used the thermal-hydraulics code as the
master and the neutronics code as the slave. This is usually the practice in modern reactor analysis codes. From this point forward it will be assumed that the master code is the thermal-hydraulics code and the slave is the neutrons code. The details of how the time step progresses further is discussed in the following several paragraphs.

**Explicit Coupling**

Explicit or sometimes called marching scheme [11] is the simplest model to implement and is probably the most widely used method currently. To obtain converged results with this coupling scheme, very small time step sizes are required. The larger the time step the greater the error from the converged solution. Therefore, for large time step sizes, this method is considered the least accurate of the schemes discussed in this dissertation.

With this method the master code converges first then sends it’s parameters to the slave processes and then the slave process converges and sends data back to the master process. A new time-step size is selected by the master code and the process is repeated for each new time-step, **Figure 1-7**.

![Explicit Process Flow for Coupled Master/Slave Code System](image)

**Figure 1-7**: Explicit Process Flow for Coupled Master/Slave Code System

Examples of this type of coupling include TRACE/PARCS and RELAP5/PARCS (shown in **Figure 1-8**). **Figure 1-8** shows a more detailed coupling between the thermal-hydraulics, heat conduction equation, and the neutronics for RELAP5/PARCS. In this
example the heat conduction equations are solved first. The results are then passed to the thermal-hydraulics and neutronics equations.

**Semi-Implicit Coupling**

Semi-implicit methods have been employed that use feedback parameters from an old time-step and some from the new time-step. This type of scheme was implemented into TRAC-PF1/NEM. In this case the current time-step fluxes and powers were calculated using the current time-step thermal-hydraulic condition and the fuel rod temperatures from a previous time-step [8] [9]. This type coupling followed the natural flow of TRAC-PF1 and is consistent with the point kinetics implementation. **Figure 1-9** shows a detailed coupling for TRAC-PF1/NEM.
The disadvantage of both of these methods (explicit and semi-implicit) is that only the individual codes are converged during the time-step. The parameters being passed are not considered in the convergence criteria. Therefore, smaller time-steps have to be made to maintain accuracy of the parameters being passed. Instabilities can develop during the transient caused by the non convergence of these parameters.

**Implicit Coupling**

This type of coupling is the focus of this thesis. Up to this point this document has focused primarily on Operator Splitting (OS) or physics based splitting of the time integration. The current research in the field of reactor analysis has shown that the OS techniques can have inaccurate results and in some cases these results may look reasonable [12][13][14][15]. Therefore, the latest research is moving towards an implicit time integration scheme. In this type of coupling not only are the individual codes converged but the feedback parameters are also converged during one time-step. This method has the advantage of being the most accurate and stable since the feedback parameters are also converged. Several different methods have been implemented to address this type of coupling. Nested loops have been used to approximate implicit coupling, Jacobian-Free Newton Krylov (JFNK) methods have been used to resolve the nonlinear terms, and a
combination of these two methods has been used or investigated. One of the more promising methods and hardest to implement is the fully implicit simultaneous solution of the equations for both neutronics and fluid/temperature field equations. Each of these will be discussed in more detail in the following paragraphs.

Nested loop iteration or fixed point iteration [16] is not an implicit scheme but approximates it by adding a loop to the current marching scheme Figure 1-10. This new loop along with new convergence criteria on the feedback parameters is used to converge the solution of the neutronics and fluid/temperature field equations. This method was investigated using TRACE and PARCS [11]. In this work the neutronics and the fluid/temperature field equations were iterated until convergence was achieved at each time-step. This work also showed an increased computational cost per time-step caused by the additional iterations, however it also showed that for a small penalty in accuracy larger time-steps could be achieved. This result only showed marginal computational savings over the traditional marching scheme. The results from this work are summarized in Table 1-1. These results are encouraging since they show that an accurate solution is obtained when the two codes are converged.

Figure 1-10 : Fixed Point Iteration Process Flow for Coupled Master/Slave System
Also presented in Reference [11] is a JFNK method for resolving the nonlinear behavior of the coupling parameters. This method showed accurate results using a Newton iteration on the nonlinear feedback terms however, has a significantly larger cost per timestep. These results are summarized in Table 1-1.

<table>
<thead>
<tr>
<th>Solution Technique</th>
<th>Difference In Power (%)</th>
<th>CPU-Time for Time-Step 0.1 sec</th>
<th>Difference In Power (%)</th>
<th>CPU-Time for Time-Step 0.5 sec</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>TRAC-M</td>
<td>PARCE</td>
<td>TRAC-M</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Time (sec)</td>
<td>Ratio</td>
<td>Time (sec)</td>
</tr>
<tr>
<td>Current</td>
<td>0.153</td>
<td>69.3</td>
<td>1.0</td>
<td>296.6</td>
</tr>
<tr>
<td>Nested Loop</td>
<td>Reference</td>
<td>253.7</td>
<td>3.7</td>
<td>582.7</td>
</tr>
<tr>
<td>JFNK</td>
<td>0.0611</td>
<td>602.6</td>
<td>9.7</td>
<td>1686.7</td>
</tr>
</tbody>
</table>

In references [15] and [13] similar approaches are shown on the example of point kinetics and one-dimensional neutronics and precursor density equations. These equations are coupled to a one-dimensional single phase flow thermal-hydraulics model. In the first paper a fixed point iteration is applied to the equation set as well as a solution method based on explicit higher order representation of the nonlinear terms. The results of this study showed that both methods were better capable of resolving the nonlinear terms. In the second paper an Implicit Runge Kutta (IRK) method was used to resolve the nonlinear feedback between the point reactor kinetics equations with feedback. This method also served well to preserve higher order accuracy for the nonlinear problem.

The implicit coupling techniques that have been discussed up to this point are considered synthetic methods for obtaining a second order accurate (in time) implicit solution. These techniques have their advantages and disadvantages and can be used in situations where one may not have access to source code. However, recent research has been moving in the direction of more formal implicit time integration techniques. The following paragraphs summarize the state-of-the-art research in this area.
In references [17][18] a Newton-BICGSTAB solver was used to resolve the non-linearities in the FORMOSA-B boiling water reactor core simulator. This method was used to evaluate the three-dimensional two-group neutron diffusion equations coupled with a three equation drift flux model. This method used a physics based preconditioner to the BICGSTAB solver and was shown to be an efficient method for steady state calculations. This research also compared the inexact Newton method to the exact Newton method and showed further speedups using the inexact method.

Some of the most advanced work in this area is presented in References [19][20]. This work presented a model consisting of nine nonlinearly coupled partial differential equations, one dimensional two-phase flow equation, a two-dimensional heat conduction equation, and a two-dimensional neutron diffusion equation with two-dimensional precursor concentration. It compared two different solution methods for solving this equation set. The traditional Operator Splitting (OS) technique and a JFNK for solving the entire set of nonlinear equations simultaneously. A physics-based preconditioner is used for the Newton-Krylov method to improve convergence. The JFNK method is fully implicit and therefore used a dynamic time-step size. The time-step decreased as the transient moved faster and the time step increased when the transient varied slowly. On the other hand the OS method was limited by the material courant limit. Both of these solution methods were used to analyze a rod ejection transient. This transient was characterized by two power spikes. One initial spike during the rod ejection and one smaller broader spike later in the transient. The results from this analysis show that the OS method approach the JFNK method as the time step size is reduced. It also showed that for similar accuracy in results the JFNK method converged at time steps 100 to 10,000 times larger than the OS method. This is by far the strongest support for the work that is proposed in this document.

1.4 Summary

This chapter introduced the basic concepts necessary to understand the methods presented in this thesis as well as a comprehensive literature survey of the current research in
this area. It showed the need in reactor analysis for improved temporal coupling of multi-
physics codes and laid the ground work for the methods proposed in Chapter 4. It shows
that the current methods for temporal coupling are limited and more advanced methods
are required to restore higher order accuracy between the coupled code systems.
Chapter 2

CURRENT SOLUTION METHODS USED BY TRACE/PARCS

This chapter will discuss the nodal balance equations and their corresponding solution as it applies to the Purdue Advanced Reactor Core Simulator (PARCS) and will contain a brief discussion of the TRAC RELAP Advanced Computational Engine (TRACE) Two-Phase Computational Fluid Dynamics (CFD) six-equation model. The current method of coupling these two computer codes is presented as well as some initial timing studies on the effect of time-step size on the TMI MSLB and the PB TT benchmark problems.

2.1 Core Physics Calculations

The goal of a core physics calculation is to predict the neutron population or change in population at any given time during the operation of the reactor or during a transient event. A transient event is one in which the thermal hydraulic conditions or power do not stay constant. When they are constant the reactor is said to be in a steady state. In reactor safety analysis two types of core physics problems are solved, the fixed source and the eigenvalue problems. The fixed source problem solves the time dependent neutron balance equations to obtain transient results for the core physics calculations. The eigenvalue problem is solved using time independent neutron balance equation. This type of calculation is generally used to initialize the power distribution before a transient calculation is performed. There are two main equations that govern the neutron population in the reactor core. Equation (2-1) is the energy dependent neutron diffusion equation and Equation (2-2) is the precursor concentration balance equation [21][22][23]. These two equations describe neutron transport and the production of neutrons from the fission reaction and decay of precursors. The subscripts p and d denote prompt and delayed neutrons respectively and l refers to the delayed precursor groups.
The energy spectrum of neutrons ranges from 10 MeV down to less than .01 eV. The energy spectrum has a complex structure which makes it unrealistic to treat the entire energy range in practical applications. It is common practice to treat the energy dependence as discrete groups and assume that the neutron properties are equivalent to the average over that energy group. The multi-group forms of equations (2-1) and (2-2) can be derived by integrating over each energy group such that as shown in Equations (2-4) and (2-5).

\[
\frac{1}{v(E)} \frac{\partial}{\partial t} \phi(\vec{r}, E, t) = \int_0^{\infty} dE \Sigma_s(E' \rightarrow E) \phi(\vec{r}, E, t) + \chi_p(E)(1 - \beta) \int_0^{\infty} dE' v_p(E') \Sigma_f(E') \phi(\vec{r}, E', t) + \chi_d(E) \sum_l \lambda_l C_l(\vec{r}, t) - \nabla \cdot \dot{J}(\vec{r}, E, t) - \Sigma_s(E) \phi(\vec{r}, E, t)
\]

\[
\frac{\partial C_l}{\partial t} = \beta_l \int_0^{\infty} v_d(E) \Sigma_f(E') \phi(\vec{r}, E', t) dE' - \lambda_l C_l(\vec{r}, t)
\]

\[
\beta_l = \sum_i \beta^i_l
\]

\[
\int_{E_g}^{E_{g-1}} \frac{1}{v(E)} \phi(\vec{r}, E, t) dE = \int_{E_g}^{E_{g-1}} dE \int_0^{\infty} dE' \Sigma_s(E' \rightarrow E) \phi(\vec{r}, E', t) + \int_{E_g}^{E_{g-1}} \chi_p(E)(1 - \beta) dE' \int_0^{\infty} dE' v_p(E') \Sigma_f(E') \phi(\vec{r}, E', t) + \int_{E_g}^{E_{g-1}} \chi_d(E) dE \sum_l \lambda_l C_l(\vec{r}, t) - \nabla \cdot \int_{E_g}^{E_{g-1}} \dot{J}(\vec{r}, E, t) dE - \int_{E_g}^{E_{g-1}} \Sigma_l(E) \phi(\vec{r}, E, t) dE
\]
Following the definitions for the group flux, total cross section, neutron speed, scattering cross section, and fission terms in references [21][23][22], the resulting energy group equations are (2-6) and (2-7). In this equation the \( g \) represent each individual energy group and \( G \) is the total number of energy groups.

\[
\frac{1}{v_g} \frac{\partial}{\partial t} \phi_g(\vec{r}, t) = \sum_{g=1}^{G} \left[ \frac{\Sigma_{sg}}{v_g} \phi_g(\vec{r}, t) + \lambda_{pg} (1 - \beta) \sum_{g=1}^{G} v_{pg} \Sigma_{fg} \phi_g(\vec{r}, t) \right] \\
+ \frac{\chi_{dg}}{v_{dg}} \sum_{l} \lambda_l C_l(\vec{r}, t) - \nabla \cdot \vec{J}_g(\vec{r}, t) - \Sigma_{fg} \phi_g(\vec{r}, t)
\]

\[
\frac{\partial C_l}{\partial t} = \beta_l \sum_{g=1}^{G} v_{dg} \Sigma_{fg} \phi_g(\vec{r}, t) - \lambda_l C_l(\vec{r}, t)
\]

The next step in the derivation of the nodal balance neutron diffusion equation is the discretization of the group equations in space. This is done by breaking up the core into smaller sections called nodes. Each node (in cartesian coordinates) is generally the size of a fuel rod bundle assembly in the x-y direction and some small portion of the axial length of the fuel rods in the z direction (typically about 15 cm). It is assumed that all parameters are constant in the node volume. With this assumption we can say that for each node volume the average neutron flux or cross section is defined as the integral over the volume divided by the total volume of the node. Equation (2-8) shows the definition for the average flux for node \( m \), the rest of the node average parameters can be determined in a similar manner. The net current formulation is a little different however. The current is a node edge value so it has to be integrated over the surface of each face of the node and then divided by the total surface area.
From equations (2-6) and (2-7) we get our time dependent nodal balance equations. This formulation is consistent with the form used in PARCS. The eigenvalue $k_{eff}$ is introduced into these equations to account for transients that start from a noncritical initial state. This eigenvalue stays constant throughout the transient and is typically determined by an initial steady state eigenvalue calculation [24].

$$\phi^m = \frac{1}{V^m} \int \phi(\mathbf{r}, t) d\mathbf{r}^3$$  \hspace{1cm} (2-8)

Figure 2-1: One Dimensional Neutronics Node

$$\frac{1}{v_g^m} \frac{d\phi_g^m}{dt} = \frac{1}{k_{eff}} \chi_{pg}(1 - \beta) \sum_{g=1}^{G} v_{pg} \Sigma_{fg}^m \phi_g^m + \chi_{dg} \sum_{l} \lambda_l C_l^m + \sum_{g'=1}^{G} \Sigma_{g'g}^m \phi_g^m$$  \hspace{1cm} (2-9)

$$- \sum_{u=x,y,z} \frac{1}{h_u^m} (J_{gu}^{m+1/2} - J_{gu}^{m-1/2}) - \Sigma_{fg}^m \phi_g^m$$

$$\frac{\partial C_l}{\partial t} = \frac{1}{k_{eff}} \beta_l \sum_{g=1}^{G} v_{dgl} \Sigma_{fg}^m \phi_g^m(t) - \lambda_l C_l^m(t)$$  \hspace{1cm} (2-10)
The steady state form of equations (2-9) and (2-10) is obtained by ignoring the time dependence in the Left Hand Side (LHS) of equations (2-9) and (2-10). Since there is no time dependence there is also no need to distinguish between prompt and delayed neutrons. These two equations collapse into one equation (2-11).

\[ \sum_{g' = 1}^{G} \Sigma_{g'} m \phi_{g}^{m} - \sum_{u = x, y, z} \frac{1}{h_{u}} \left( J_{gu}^{m+1/2} - J_{gu}^{m-1/2} \right) - \Sigma_{f g} m \phi_{g}^{m} = \frac{1}{k_{\text{eff}}} \chi_{g} \sum_{g = 1}^{G} v_{g} \Sigma_{f g}^{m} \phi_{g}^{m} \]  

(2-11)

### 2.1.1 PARCS Solution to the Eigenvalue Problem

The purpose of the eigenvalue problem is to perform a critically search on equation (2-11). That is, given the geometry and the fission source, calculate \( k_{\text{eff}} \) and the neutron flux. PARCS uses the Wielandt shift method to determine the flux and eigenvalue of the system [25]. The first step is to rewrite equation (2-11) in operator form (2-12). This will make manipulation of the equation much easier.

\[ M \phi = \frac{1}{k_{\text{eff}}} F \phi \]  

(2-12)

where:

\[ M = \sum_{g' = 1}^{G} \Sigma_{g'} m \phi_{g}^{m} - \sum_{u = x, y, z} \frac{1}{h_{u}} \left( J_{gu}^{m+1/2} - J_{gu}^{m-1/2} \right) - \Sigma_{f g} m \phi_{g}^{m} = \text{Migration Matrix} \]

\[ F = \chi_{g} \sum_{g = 1}^{G} v_{g} \Sigma_{f g}^{m} \phi_{g}^{m} = \text{Fission Matrix} \]

The Wielandt shift method involves subtracting a fission source term from both sides of equation (2-12) and recasting the problem. The new fission source term is calculated
by perturbing the original eigenvalue by $\delta k$. Equation (2-13) defines the new fission source term and equation (2-16) is the final version of the recast problem.

$$F_s = \frac{1}{k_s} F$$  \hspace{1cm} (2-13)

Where $k_s = k_{\text{eff}} + \delta k$

$$(M - F_s) \phi = (F - F_s) \phi$$  \hspace{1cm} (2-14)

Let $A = M - F_s$ and $\frac{1}{k_A} = \frac{1}{k_{\text{eff}}} - \frac{1}{k_s}$  \hspace{1cm} (2-15)

$$A \phi = \frac{1}{k_A} F \phi$$  \hspace{1cm} (2-16)

Equation (2-16) can be solved using the power method. This is done by taking an initial guess at the fission source term in equation (2-16), $F_\phi = S$. With this initial guess and using equation (2-16), the flux can be solved for. Once the flux is known the fission source can be solved for explicitly. This processes will continue until the flux and the eigenvalue converge. The iterative equations are shown in equations (2-17) and (2-18).

$$A^{(n+1)} = \frac{1}{k_A^{(n)}} S^{(n)}$$  \hspace{1cm} (2-17)

$$S^{(n)} = F_\phi^{(n)}$$  \hspace{1cm} (2-18)

The iteration scheme given by equation (2-17) the eigenvalue are updated using the relation given in equation (2-19).

$$k_A^{(n+1)} = k_A^{(n)} \frac{\langle S^{(n+1)}, S^{(n+1)} \rangle}{\langle S^{(n+1)}, S^{(n)} \rangle}$$  \hspace{1cm} (2-19)
2.1.2 PARCS Solution to the Fixed Source Problem

This section will show the PARCS solution to the transient fixed source problem represented by equations (2-9) and (2-10). To solve these equations there are typically several assumptions and simplifications made. PARCS solves these equations first assuming two energy groups. The second assumption that is made is that all fission neutrons, both prompt and delayed are born in energy group 1, that is they are all fast fission neutrons \( \chi_{p1} = \chi_{d1} = 1.0, \chi_{p2} = \chi_{d2} = 0.0 \). The third assumption is the delayed precursor density is not dependent on the incident neutron energy. The fourth assumption is \( v_{dg1} \Sigma_{fg} = \beta_1 v_{\Sigma_{fg}} \) and \( v_{pg1} \Sigma_{fg} = (1 - \beta)v_{\Sigma_{fg}} \), and the fifth assumption is, there is no scattering from a lower energy group to a higher energy group. With these assumptions equations (2-9) and (2-10) can be written in the two-group form, equations (2-20), (2-21), and (2-22).

Fast Group, \( g = 1 \):

\[
\frac{1}{v_1} \frac{d\phi_1^m}{dt} = \frac{1}{k_{eff}} (1 - \beta^m) (v\Sigma_{fg1}^m \phi_1^m + v\Sigma_{fg2}^m \phi_2^m) + \sum_l \lambda_l C_l^m - \sum_{u-s,x,z} h_u^m (J_{1u}^{m+1/2} - J_{1u}^{m-1/2}) - \Sigma_{R1}^m \phi_1^m
\]  
(2-20)

Thermal Group, \( g = 2 \):

\[
\frac{1}{v_2} \frac{d\phi_2^m}{dt} = \Sigma_{s1}^m 2\phi_1^m - \sum_{u-s,x,z} h_u^m (J_{2u}^{m+1/2} - J_{2u}^{m-1/2}) - \Sigma_{R2}^m \phi_2^m
\]  
(2-21)

\[
\frac{\partial C_l}{\partial t} = \frac{1}{k_{eff}} \beta_l^m (v\Sigma_{fg1}^m \phi_1^m + v\Sigma_{fg2}^m \phi_2^m) - \lambda_l C_l^m(t)
\]  
(2-22)

In order to solve equations (2-20), (2-21), and (2-22) with a computer we need to discretize these equations in time. The method PARCS uses to do this is the theta method. The theta method acts as a weighting factor between the time levels \( n \) and \( n-1 \), as shown in
equation (2-23). If \( \theta = 0 \), this method reduces to a forward Euler or explicit time integration method, if \( \theta = 1 \), the method reduces to the backward Euler or implicit time integration method. PARCS uses a value of \( \theta = 1/2 \), which is second order accurate Crank-Nicolson Scheme [24].

Let: 
\[
R_g^m = \frac{1}{k_{\text{eff}}} \chi_{pg} \sum_i (1 - \beta_i) \sum_{g=1}^G \nu_{pg} \Sigma_f^m \phi_g^m + \chi_{dg} \sum_l \lambda_l \Sigma_C^{lm} + \sum_{g'=1}^G \Sigma_{g'g} \phi_g^m
\]

\[
- \sum_{u=x,y,z} h_u \left( J_{gu}^{m+1/2} - J_{gu}^{m-1/2} \right) - \Sigma_{ig} \phi_g^m
\]

Then: 
\[
\frac{1}{v_g^m} \frac{d\phi_g^m}{dt} = R_g^m \frac{\phi_g^{m,n+1} - \phi_g^{m,n}}{v_g^m \Delta t} = \theta R_g^{m,n+1} + (1 - \theta) R_g^{m,n} \quad (2-23)
\]

Figure 2-2 : One Dimensional Three Neutronics Nodes

\[
J_{g,u}^{m+1/2} = -\tilde{D}_{g,u}^{m+1/2} (\phi_g^{m+1} - \phi_g^m) - \tilde{D}_{g,u}^{m+1/2} (\phi_g^{m+1} + \phi_g^m) \quad (2-24)
\]

\[
J_{g,u}^{m-1/2} = -D_{g,u}^{m-1/2} (\phi_g^{m-1} - \phi_g^m) - D_{g,u}^{m-1/2} (\phi_g^{m-1} + \phi_g^m) \quad (2-25)
\]

Where:
\[ \tilde{D}_{g,u}^{m \pm 1/2} = \frac{2D_{g}^{m \pm 1}D_{g}^{m}}{D_{g}^{m \pm 1} \Delta u_{m} + D_{g}^{m} \Delta u_{m \pm 1}} \quad (2-26) \]

\[ \tilde{D}_{g,u}^{m \pm 1/2} \] is called the base coupling coefficient. It represents a first order finite difference approximation to the coupling of node \( m \) to node \( m \pm 1 \). The \( \tilde{D}_{g,u}^{m \pm 1/2} \) term is called the Corrective Nodal Coupling Coefficient (CNCC). This term corrects the interfacial nodal currents shown in equation (2-24), to be consistent with the currents calculated using a higher order technique. In PARCS this is done by solving a two node problem with the Analytic Nodal Method (ANM). The details of ANM are not discussed in this thesis. A complete description can be found in [24].

The precursor balance equation (2-22) is also time dependent. Instead of discretizing this equation with time, an analytic solution is used. It is assumed that the variation of the fission source over the time interval \( \Delta t_{n} \) is quadratic in time. A linear assumption could also be assumed here, however PARCS chose a quadratic form since the flux variation associated with \( \theta = 0.5 \) is also second order. From this assumption the new time precursor concentration can be written in terms of old time concentrations and fluxes for any node \( m \) as shown in equation (2-27). A more detailed description is given in [24].

\[ C_{k}^{n+1} = \kappa_{k}C_{k}^{n} + \frac{\beta_{k}}{\kappa_{k}}(\Omega_{k}^{n-1}\Psi_{n-2} + \Omega_{k}^{n}\Psi_{n-1} + \Omega_{k}^{n+1}\Psi_{n}) \quad (2-27) \]

where:

\[ \Psi = \frac{1}{k_{\text{eff}}^{g}} \sum_{g=1}^{2} v \Sigma_{fg} \phi_{g} \]

\[ \gamma = \frac{\Delta t_{n+1}}{\Delta t_{n}} \]

\[ \kappa_{k} = e^{-\lambda_{k}\Delta t_{n+1}}, \kappa_{k} = 1 - \kappa_{k} \]
The role of Computational Fluid Dynamics (CFD) in reactor safety is to simulate the flow of steam-water mixture throughout the entire reactor system. This can be done with varying levels of detail from very coarse lumped parameter homogenous flow equations to very detailed Navier Stokes equations which can resolve detailed turbulent flow. TRACE solves for the two-phase fluid conditions using the six equation model. This model uses a set of mass, momentum, and energy Partial Differential Equations (PDEs) to model the steam-water flow. TRACE assumes that any non condensable gas present in the gas mixture has the same velocity and temperature as the steam in the mixture. Therefore to account for the presence of a non condensable gas only an added mass conservation equation is needed. A detailed discussion of two-phase fluid dynamics will not be presented here. We will present enough information for the reader to understand the current solution methods used by a state-of-the-art thermal hydraulics reactor analysis code.

2.2 Six Equation Model

The following equations (2-28) through (2-33) represent the six equation model. These six equations model the mass, momentum, and energy transfer between water and steam. These equations also govern the heat flow between the fluid and structure. A seventh equation (2-34) is added to model non condensable gas that may be present in the two-phase mixture.
Gas Momentum:
\[ \alpha_g \left( \frac{\partial \hat{V}_g}{\partial t} + \hat{V}_g \cdot \nabla \hat{V}_g \right) = -\alpha \nabla \hat{P} - \alpha \rho_g \hat{g} - f_i + f_{wg} \]  
(2-28)

Liquid Momentum:
\[ (1 - \alpha) \rho_l \left( \frac{\partial \hat{V}_l}{\partial t} + \hat{V}_l \cdot \nabla \hat{V}_l \right) = - (1 - \alpha) \nabla \hat{P} - (1 - \alpha) \rho_l \hat{g} + f_i - f_{wl} \]  
(2-29)

Gas Mass:
\[ \frac{\partial \alpha \rho_g}{\partial t} + \nabla \cdot (\alpha \rho_g \hat{V}_g) = \Gamma_i \]  
(2-30)

Liquid Mass:
\[ \frac{\partial (1 - \alpha) \rho_l}{\partial t} + \nabla \cdot [(1 - \alpha) \rho_l \hat{V}_l] = -\Gamma_i \]  
(2-31)

Mixture Energy:
\[ \frac{\partial}{\partial t} \left[ \alpha \rho_g e_g + (1 - \alpha) \rho_l e_l \right] + \nabla \cdot \left[ \alpha \rho_g e_g \hat{V}_g + (1 - \alpha) \rho_l e_l \hat{V}_l \right] = \]  
\[ - P \nabla \cdot [\alpha \hat{V}_g + (1 - \alpha) \hat{V}_l] + q_{wg} + q_{wl} + q_{dg} + q_{dl} \]  
(2-32)

Gas Energy:
\[ \frac{\partial}{\partial t} (\alpha \rho_g e_g) + \nabla \cdot (\alpha \rho_g \hat{V}_g) = - P \left[ \frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \hat{V}_g) \right] + \Gamma h_{fg} + q_{wg} + q_{ig} + q_{dg} \]  
(2-33)

Non Condensable Gas:
\[ \frac{\partial \alpha \rho_a}{\partial t} + \nabla \cdot (\alpha \rho_a \hat{V}_g) = 0 \]  
(2-34)

Equations (2-28) through (2-34) are spatially discretized using a finite volume method. TRACE uses a staggered mesh technique where static variables such as the thermodynamic state variables are evaluated at the volume center and the fluid velocities are evaluated at the volume surface. Figure 2-3 shows a typical staggered mesh used to
develop the discrete finite volume equations for TRACE. The computational volumes are represented by the solid black lines. These volumes are used to develop the discrete mass and energy equations. However, the discrete momentum equations are developed using the momentum volume shown by the dashed line. Equations (2-28) through (2-34) are linearized using total pressure, void fraction, liquid and gas temperature, and non-condensable gas pressure. Other quantities required to solve equations (2-28) through (2-34), like density, liquid and gas internal energies are calculated by the equation of state as functions of temperature and pressure.

The time derivatives in equations (2-28) through (2-34) are evaluated using a semi-implicit time integration method. TRACE evaluates quantities associated with a pressure wave propagation at new time values. Therefore, the pressure gradient in the momentum equation is evaluated at the new time values as shown in equation (2-35). The time derivatives for the each of the terms given in equations (2-28) through (2-34) are approximated using equation (2-36).
Where $\Psi$ represents the term or terms that the partial derivative is being taken. The semi-implicit time discretization of the six-equation model are given in equations (2-40) through (2-46). The wall drag and interfacial drag terms given in equations (2-28) and (2-29) are represented in discrete form as follows:

\begin{align*}
\frac{dP}{dx} & \approx \frac{P_{j+1}^{n+1} - P_j}{\Delta x_{j+1/2}} \\
\frac{\partial \Psi}{\partial t} & \approx \frac{\Psi_{j}^{n+1} - \Psi_j^n}{\Delta t}
\end{align*}

(2-35)  
(2-36)

A more detailed derivation of these equations can be found in [3]. The velocity derivative in the flux momentum term is left in its differential form for simplicity. The spatial subscript $j + 1/2$ has been left off of the Velocity terms as well. All velocities without a subscript are assumed to be at $j + 1/2$. 

\begin{align*}
f_{wg} &= C_{wg} V_g |V_g| = \frac{C_{wg}}{(\alpha \rho_g)_{j+1/2}^n} (2V_g^{n+1} - V_g^n) |V_g^n| \\
f_{wl} &= C_{wl} V_i |V_i| = \frac{C_{wl}}{(1-\alpha \rho_l)_{j+1/2}^n} (2V_i^{n+1} - V_i^n) |V_i^n| \\
f_i &= C_i (V_g - V_i) |V_g - V_i| = \frac{C_i}{(\alpha \rho_g)_{j+1/2}^n} \left[ (V_g^n + V_i^{n+1}) - (V_g^n - V_i^n) \right]
\end{align*}

(2-37)  
(2-38)  
(2-39)
\[
\frac{V_{g}^{n+1} - V_{g}^{n}}{\Delta t} + V_{g}^{n+1} \frac{\partial V_{g}^{n}}{\partial x} = \frac{1}{\langle \rho_{g}^{n+1} \rangle} \frac{(P_{j+1}^{n+1} - P_{j}^{n+1})}{\Delta x_{j+1/2}} \\
+ \frac{\Gamma_{i+1/2}^{n+1}}{\langle \rho_{g}^{n+1} \rangle} (V_{g}^{n+1} - V_{l}^{n+1}) \quad (2-40)
\]

\[
\frac{V_{l}^{n+1} - V_{l}^{n}}{\Delta t} + V_{l}^{n+1} \frac{\partial V_{l}^{n}}{\partial x} = \frac{1}{\langle \rho_{l}^{n+1} \rangle} \frac{(P_{j+1}^{n+1} - P_{j}^{n+1})}{\Delta x_{j+1/2}} \\
- \frac{\Gamma_{i+1/2}^{n+1}}{\langle (1 - \alpha) \rho_{l}^{n} \rangle} (V_{l}^{n+1} - V_{g}^{n+1}) \quad (2-41)
\]

\[
\frac{\alpha_{j}^{n+1} \rho_{gj}^{n+1} - \alpha_{j}^{n} \rho_{gj}^{n}}{\Delta t} + \nabla_{j} \cdot [\alpha^{n} \rho_{g}^{n} V_{g}^{n+1}] = \Gamma_{j}^{n+1} \quad (2-42)
\]

\[
\frac{[(1 - \alpha_{j}^{n+1}) \rho_{lj}^{n+1} - (1 - \alpha_{j}^{n}) \rho_{lj}^{n}]}{\Delta t} + \nabla_{j} \cdot [(1 - \alpha^{n}) \rho_{l}^{n} V_{l}^{n+1}] = -\Gamma_{j}^{n+1} \quad (2-43)
\]

\[
\frac{[\alpha_{j}^{n+1} \rho_{aj}^{n+1} - \alpha_{j}^{n} \rho_{aj}^{n}]}{\Delta t} + \nabla_{j} \cdot [\alpha^{n} \rho_{a}^{n} V_{g}^{n+1}] = 0 \quad (2-44)
\]

\[
\frac{[\alpha_{j}^{n+1} \rho_{gj}^{n+1} e_{gj}^{n+1} - \alpha_{j}^{n} \rho_{gj}^{n} e_{gj}^{n}]}{\Delta t} + \nabla_{j} \cdot [\alpha^{n} \rho_{g}^{n} e_{g}^{n} V_{g}^{n+1}] \\
+ p^{n+1} \left[ \frac{(\alpha^{n+1} - \alpha^{n})}{\Delta t} + \nabla_{j} \cdot (\alpha^{n} \rho_{g}^{n+1}) \right] \\
= q_{wg}^{n+1} + q_{dg}^{n} + q_{lg}^{n+1} + \Gamma_{n+1} h_{sg}^{n+1} \quad (2-45)
\]
The interfacial mass transfer rate, the wall heat transfer to the liquid and gas phases, and the interfacial heat transfer are defined as:

\[
\frac{[\alpha_j^n + 1 \rho_{gl}^{n+1} e_{lj}^{n+1} + (1 - \alpha_j^n) \rho_{lj}^{n+1} e_{lj}^{n+1}]}{\Delta t} - \frac{\alpha_j^n \rho_{gl}^n e_{lj}^n + (1 - \alpha_j^n)(\rho_{lj}^n e_{lj}^n)}{\Delta t} + \nabla_j \cdot \left[ \alpha^n \rho_g^n e_g^n V_g^{n+1} + (1 - \alpha^n) \rho_l^n e_l^n V_l^{n+1} \right] + P^{n+1} \nabla_j \cdot \left[ (1 - \alpha) V_l^{n+1} + \alpha V_g^{n+1} \right] = q_{wg}^{n+1} + q_{wl}^{n+1} + q_{dl}^n + q_{dg}^n
\]

The interfacial mass transfer rate, the wall heat transfer to the liquid and gas phases, and the interfacial heat transfer are defined as:

\[
\Gamma_{n+1} = \frac{-(q_{lg}^{n+1} + q_{li}^{n+1})}{(h_v^l)^{n+1} - (h_i^l)^{n+1}}
\]

\[
q_{wl}^{n+1} = h_{wl} a_w (T_w^{n+1} - T_l^{n+1})
\]

\[
q_{wg}^{n+1} = h_{wg} a_w (T_w^{n+1} - T_g^{n+1})
\]

\[
q_{ig}^{n+1} = h_{ig} a_i (T_{sat}^{n+1} - T_g^{n+1})
\]

\[
q_{li}^{n+1} = h_{li} a_i (T_{sat}^{n+1} - T_l^{n+1})
\]

Of particular importance to this thesis is the heat transfer coefficients for the heat transfer to the liquid and the gas phases. These values are calculated at old time values and were implemented in this fashion for simplicity. However, bounded instabilities can occur during calculations.

This thesis only utilizes the semi-implicit method for developing the discrete fluid equations. TRACE also has another method called the Stability-Enhancing Two-Step (SETS) scheme, the details of which will not be presented here. This method is a predictor-corrector method based on the semi-implicit method. An additional corrector (stabi-
lizer) step is added to calculate the new time densities. By doing this the material courant time step limit can be exceeded. This method is not unconditionally stable and can add error from numerical diffusion to some calculations [3]. This has been seen in resent studies for BWR stability problems. This method will not be used for any of the work proposed in this document. The details presented in this section should be sufficient for the reader to have a basic understanding of the fluid equations used in TRACE.

2.3 TRACE Heat Conduction

The heat conduction model in TRACE is used to represent the transfer of heat between the reactor structure and the fluid in the reactor. The heat conduction model used in TRACE is capable of modeling cylindrical wall, slabs, and core fuel rods. These really represent two different heat conduction models. One for the cylindrical wall geometry and one for the slabs and fuel rods. Only the second model for the rod and slab have a direct application to the coupling proposed later in this thesis. This section will present a brief overview of the current rod and slab models as they are implemented in TRACE.

The heat conduction in a solid material with a generic geometry can be described using equation (2-52).

\[
\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q'''
\]  

(2-52)

2.3.1 Rod and Slab Heat Conduction

The semi-implicit finite difference formulation for the heat conduction equation is obtained by applying the integral method to differential volumes. Similar to the methods used for generating the finite difference formulations for the neutronics equations and the thermal-hydraulic equations. The semi-implicit representation uses implicit differencing in the radial direction and an explicit differencing in the axial direction. Figure 2-4 shows
a general representation for the heat conduction in the fuel, gap, and cladding. Using the general volume labeled $i,j$ the finite difference form of equation (2-52) is [3]:

$$
\left\{ \left( \rho c_p \right)_{ij} \frac{T_{ij}^{n+1} - T_{ij}^n}{\Delta t} - q_{ij}^n \right\} \frac{1}{2} \left[ T_{ij}^n + \frac{\Delta r_i^2}{4} \right] + \left[ T_{ij}^n - \frac{\Delta r_i^2}{4} \right] \frac{r_{ij}^n}{\Delta z_j^* + \Delta z_{j-1}^*} \\
= \left\{ r_{i+1/2,j+1/2} \frac{T_{i+1,j}^{n+1} - T_{ij}^n}{\Delta r_i} \right\} + \left\{ r_{i-1/2,j-1/2} \frac{T_{i-1,j}^{n+1} - T_{ij}^n}{\Delta r_i} \right\} \\
\times \left[ \frac{\Delta z_j + \Delta z_{j-1}}{2} \right] + \left\{ k_{i,j+1/2} \frac{T_{i,j+1}^n - T_{ij}^n}{\Delta z_j} \right\} + \left\{ k_{i,j-1/2} \frac{T_{i,j-1}^n - T_{ij}^n}{\Delta z_j} \right\} \\
\times \left[ \frac{1}{2} \left[ r_{ij}^n \frac{\Delta r_i^2}{4} + r_{ij}^n \frac{\Delta r_i^2}{4} \right] \right]
$$

(2-53)

![Figure 2-4: Heat Conduction Volumes for the Fuel Rod](image)

The transport of heat between the liquid or vapor and the heat structure wall is modeled using Newton’s law of cooling. The rate at which heat is exchanged between the fuel and the fluid is dependant on the flow regime model that is used to calculate the heat trans-
fer coefficients (HTC). Because of this the coupling of the heat conduction to the fluid equations is implicit in terms of the wall, liquid, and vapor temperatures but explicit in terms of the HTCs. The total energy transported to the fluid cell from the fuel is then given by equation (2-54).

\[ q_{\text{total}}^{n+1} = h_i^n(T_w^n - T_i^n) + h_g^n(T_w^n - T_g^n) + \]
\[ \left[ h_i^n\left(\frac{\partial T_w}{\partial T_i} - 1\right) + h_g^n\frac{\partial T_w}{\partial T_g}\right](T_i^n + 1 - T_i^n) + \left[ h_g^n\left(\frac{\partial T_w}{\partial T_g} - 1\right) + h_i^n\frac{\partial T_w}{\partial T_i}\right](T_g^n + 1 - T_g^n) \]

2.3.2 Current coupling

The current coupling method used by the production version of TRACE and PARCS is the explicit marching technique shown in Figure 1-7. The propagation of data between the neutronics, thermal-hydraulics, and fluid equations is show in Figure 2-5. This current coupling technique is very sensitive to both the spatial coupling and the temporal coupling. The following paragraphs demonstrate the sensitivity to time step size for two problems, the OECD/NRC Three Mile Island (TMI) Main Steam Line Break (MSLB) benchmark problem[27] and the OECD/NRC Peach Bottom (PB) Turbine Trip (TT) benchmark problem[27]. Both of these benchmark problems are well established coupled code problems.
Three Mile Island Main Steam Line Break

This benchmark is based on real plant design and operational data for the TMI unit 1 Nuclear Power Plant (NPP). The purpose of this benchmark is three-fold: to verify the capability of system codes for analyzing complex transients with coupled core-plant interactions; to test fully the 3D neutronics/thermal-hydraulics coupling; and to evaluate discrepancies among the predictions of coupled codes in best-estimate transient simulations. The purposes of the benchmark are met through the application of three exercises: a point kinetics plant simulation (Exercise 1), a coupled 3D neutronics/thermal-hydraulics evaluation of core response (Exercise 2), and a best-estimate coupled core-plant transient model (Exercise 3).

The initiating event of the MSLB is assumed to be a double-ended rupture of one steam line upstream of the main steam isolation valve (MSIV) at the cross-connect. The loss of the secondary coolant causes a decrease in steam pressure and an increase of steam flow through the steam generator (SG) connected to the ruptured steam line. The higher steam flow rate increases the heat transfer from the primary to the secondary side and results in lower coolant temperature in the loop of the broken steam line. Because of the large negative moderator temperature coefficient, the lower coolant temperature in half of
the core region causes a positive reactivity insertion in this part of the core and consequently a power increase. The reactor is tripped because of either too low reactor coolant pressure or high neutron flux. Following the reactor trip, the turbine trips and the turbine stop valves and feed water control valves close. The low steam line pressure initiates the automatic feed water isolation, which causes the SG associated with the rupture to blow dry. The high-pressure injection (HPI) system may be activated by low reactor coolant system (RCS) pressure during the cool down period following a large area steam line break.

One of the major concerns for the MSLB is the return to criticality and/or return to power in the second half of the transient. To maximize the conservative conditions for the return to power, the MSLB transient is assumed to take place at hot full power (HFP) operating conditions at the end of cycle (EOC). The limiting MSLB for TMI-I is at HFP because the SG liquid inventory increases as the power level increases: the worst case over cooling occurs at the maximum power level, which corresponds to the maximum liquid inventory in the SG.

Another conservative assumption is that the control rod with the maximum worth is stuck in a fully withdrawn position throughout the transient. This is a limiting condition because it reduces the available scram worth even further, and increases the probability of a return to power.

This benchmark had 25 participants representing 11 countries. The results submitted by the participants for each exercise are used to make code-to-code comparisons and a subsequent statistical analysis. The results encompass several types of data for both thermal-hydraulics and neutronics parameters at the initial steady state conditions and throughout the MSLB transient [26][27][28]. Figure 2-6 and Figure 2-7 show the range in solutions from the participants. There are many causes for the differences in the participants results some of which can be attributed to temporal coupling.
Figure 2-8 shows the study I preformed on the sensitivity of the MSLB benchmark to time step size as analyzed with the current coupling of TRACE/PARCS. The core average
total power history is plotted for this event. A study was performed to see how this transient would respond to changes in time step size. From this figure we can see that as the maximum time step is increased the transient response is delayed. **Figure 2-9, Figure 2-10, and Figure 2-11** are blowups of the sections of the power curve marked in **Figure 2-8**.

![Figure 2-8: TMI MSLB Reactor Power Time-Step Sensitivity](image)
Figure 2-9 : Blowup of Section A from Figure 2-8

Figure 2-10 : Blowup of Section B from Figure 2-8
Peach Bottom Turbine Trip

Following the success of the PWR MSLB benchmark another OECD/NRC sponsored coupled code benchmark was defined for a BWR TT transient. Turbine trip transients in a BWR are pressurization events in which the coupling between core space-dependent neutronic phenomena and system dynamics plays an important role. In addition, the available real plant experimental data makes this benchmark problem very valuable. Over the course of defining and coordinating the BWR TT benchmark, the systematic validation approach, established during the PWR MSLB benchmark, was further developed to study different numerical and computational aspects of coupled best-estimate simulations.

Three TT transients at different power levels were performed at the PB-2 NPP (a GE BWR/4) prior to shutdown for refuelling at the end of Cycle 2 in April 1977. The second test (TT2) has been selected for the benchmark problem since it has the highest quality measured data set in order to investigate the effect of the pressurization transient (which follows the sudden closure of the turbine stop valve) on the neutron flux in the reactor.

Figure 2-11: Blowup of Section C from Figure 2-8
The tests were designed to produce plant/core responses that approached the design basis conditions as closely as possible. The actual data were collected, including a compilation of reactor design and operating data for Cycles 1 and 2 and the plant transient experimental data. This transient was selected for this benchmark study because it is a dynamically complex event with reactor variables changing very rapidly, and it constitutes a good problem to test the coupled codes on both levels: neutronics/thermal-hydraulics coupling, and core/plant system coupling. In the TT2 test, the thermal-hydraulic feedback alone limited the power peak and initiated the power reduction. The void feedback plays the major role while the Doppler feedback plays a subordinate role. The reactor scram then inserted additional negative reactivity and completed the power reduction and eventual core shutdown. Figure 2-12 illustrates the measured time history data of the core neutron flux and total reactivity. This provides a unique opportunity for a comprehensive feedback testing and examination of capability of advanced codes to analyze complex transients with coupled core/plant interactions through comparison with actual experimental data [27][29].

Figure 2-12 : PB TT Reactor Power Time-Step Sensitivity
A similar sensitivity study to the MSLB, was performed with this calculation as well using the current coupling of TRACE/PARCS. Figure 2-13 and Figure 2-14 show the impact of time step size on the peak power predicted in this problem. As the time step size is increased the peak power decreases.

![Figure 2-13: PB TT Reactor Power Time-Step Sensitivity](image)

Figure 2-13 : PB TT Reactor Power Time-Step Sensitivity
In this chapter, the current solution methods for the governing equations of TRACE and PARCS are presented. Sufficient detail was used to understand the equations and solutions methods for the TRACE six-equation model, TRACE heat conduction, and the PARCS neutron balance equations. Also presented in this chapter is the current coupling between TRACE and PARCS. A study was performed using the existing coupling to demonstrate the sensitivity of the current method to time-step size. This study showed that the two OECD/NRC benchmark problems chosen are sensitive to changes in time-step size and are good candidates for the evaluation of the method proposed in this document.

2.4 Summary

Figure 2-14: Blowup of section A from Figure 2-13
Chapter 3

DESCRIPTION OF CROSS SECTION DEPENDENCES ON THERMAL-HYDRAULIC PARAMETERS

3.1 Nonlinear Cross Section Dependence on Feedback Parameters

Thus far in this document we have concentrated on the nonlinear feedback between the thermal-hydraulics and the power. It is understood that the flux is nonlinearly dependent on the cross sections due to thermal-hydraulic feedback. Of particular interest is the importance of each feedback parameter on the neutron flux. This aspect is less well known and a detailed investigation will need to be done, however, some research has been done on the nonlinear behavior of cross sections based on thermal-hydraulic feedback [30][31]. In reactor analysis there are two main methods for representing cross sections dependencies on thermal-hydraulic feedback parameters. The method most commonly used is the polynomial fitting procedure and this method is described in more detail later in this chapter. The other method involves interpolation of tabulated values. Both of these methods can be used to examine the dependences of cross sections on feedback parameters. This chapter discusses these dependences using both methods.

In the libraries for both OECD/NRC benchmarks, TMI MSLB and the PB TT, are dependent only on fuel temperature and moderator density and are stored in a manner similar to that shown in Figure 3-2. In the libraries generated for the TMI MSLB, 5 different fuel temperatures and 6 different densities were chosen to represent both the steady state and transient conditions for this particular problem. Figure 3-1 shows how the fast group absorption cross section varies with fuel temperature and moderator temperature. This figure clearly shows the nonlinear behavior of the cross section. Figure 3-3 shows a sam-
ple of the density dependence at a particular temperature. This figure also shows the range densities chosen for steady-state and transient conditions. **Figure 3-4** is a more interesting from the stand point of this thesis. It shows the same data plotted in **Figure 3-3** but as a function of total pressure and moderator temperature. This figure also shows a full range of pressure and moderator temperature combinations. It also shows how the cross sections vary with density. Because of these variations the cross sections should be functions of pressure and moderator temperature to resolve all nonlinearities, however, the current libraries for these benchmark problems are based on density alone.

![Figure 3-1: Fuel and Moderator Temperature Affects on Cross Sections](image)

**Figure 3-1**: Fuel and Moderator Temperature Affects on Cross Sections
Figure 3-2: Table Representation of Cross Sections

<table>
<thead>
<tr>
<th>$T_{m_1}$</th>
<th>$T_{m_0}$</th>
<th>$T_{m_2}$</th>
<th>$T_{m_3}$</th>
<th>$T_{m_4}$</th>
<th>$T_{m_5}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{i_1}$</td>
<td>$P_{i_2}$</td>
<td>$P_{i_3}$</td>
<td>$P_{i_4}$</td>
<td>$P_{i_5}$</td>
<td>$P_{i_6}$</td>
</tr>
<tr>
<td>$E_{i_1}$</td>
<td>$E_{i_2}$</td>
<td>$E_{i_3}$</td>
<td>$E_{i_4}$</td>
<td>$E_{i_5}$</td>
<td>$E_{i_6}$</td>
</tr>
</tbody>
</table>

Figure 3-3: Density Dependent Cross Sections

![Graph showing the relationship between group 2 fission cross sections and moderator density](image-url)

Steady State

Transient

Figure 3-3: Density Dependent Cross Sections
In traditional reactor analysis macroscopic cross sections are tabulated along with derivatives of each cross section with respect to fuel temperature $T_f$, moderator temperature $T_m$, moderator density $\rho_m$, and boron concentration $C_B$. The cross sections based on feedback are then calculated using a linear combination of these tabulated terms called a polynomial fitting procedure, equation (3-1). This method was widely used in fuel management and then extended to transient analysis. Reference [30] shows that this representation is inaccurate for transients with widely varying thermal-hydraulic conditions. In this reference a new method of generating and tabulating cross sections was developed, Advanced High-order Table Lookup Method (AHTLM), which included all of the feedback dependences of each cross section in the library. Subsequent to this work, a detailed study was done to quantify the accuracy of the cross sections and the effect of each feedback parameter on $k_\infty$. In this study $k_\infty$ was calculated based on the cross sections estimated using equation (3-1), within the PRISM computer code [32], and compared to the $k_\infty$ calculated with the actual cross sections at that state point. Equation (3-2) is the formulation for $k_\infty$ used in this analysis [33][34][35].
\[
\Sigma_x(T_f, T_m, \rho_m, C_B) = \Sigma_x(T_f, T_m, \rho_m, C_B)^{ref} + \left(\sqrt{T_f^{ref}} - \sqrt{T_f}\right) d\Sigma_x(T_f) \\
+ \left(\sqrt{T_f^{ref}} - \sqrt{T_f}\right)^2 \frac{d^2 \Sigma_x(T_f)}{2} + \left(\sqrt{T_f^{ref}} - \sqrt{T_f}\right)^3 \frac{d^3 \Sigma_x(T_f)}{6} \\
+ (T_m^{ref} - T_m)d\Sigma_x(T_m) + (T_m^{ref} - T_m) \frac{2d^2 \Sigma_x(T_m)}{2} \\
+ (T_m^{ref} - T_m) \frac{3d^3 \Sigma_x(T_m)}{6} + (\rho_m^{ref} - \rho_m)d\Sigma_x(\rho_m) \\
+ (B^{ref} - B)d\Sigma_x(B)
\]

\[
k_\infty = \frac{\Sigma_{s1}}{\Sigma_{a1} + \Sigma_{s1 \to 2}} + \frac{\Sigma_{s1 \to 2}}{\Sigma_{a1} + \Sigma_{s1 \to 2}} \frac{\Sigma_{s2}}{\Sigma_{a2}}
\]

The base cross sections and their derivatives were generated by CASMO-3 [36][37] and tabulated into a typical cross section library. Each parameter was varied to determine how accurate the polynonmial fitting procedure was to estimating the cross section. Table 3-2, Table 3-3, and Table 3-4 summarizes these results. In columns where no value is given, the value is unchanged from the reference value given in Table 3-1.

**Table 3-1: Test Matrix Reference Values**

\[
\begin{align*}
C_B &= 500 \text{ ppm} \\
T_f &= 690 ^\circ C \\
T_m &= 310 ^\circ C \\
\rho_m &= 0.70 \text{ g/cm}^3
\end{align*}
\]
### Table 3-2: Test Matrix for Comparison of Polynominal Fitting Procedure vs. CASMO

<table>
<thead>
<tr>
<th>Test #</th>
<th>C\textsubscript{s} (ppm)</th>
<th>T\textsubscript{r} (°C)</th>
<th>T\textsubscript{m} (°C)</th>
<th>P\textsubscript{m} (g/cm\textsuperscript{3})</th>
<th>k\textsubscript{m}</th>
<th>Δk\textsubscript{m} x 10\textsuperscript{5} (F-C)</th>
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### Table 3-3: Test Matrix for Comparison of Polynominal Fitting Procedure vs. CASMO

<table>
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<tr>
<th>Test #</th>
<th>C\textsubscript{s} (ppm)</th>
<th>T\textsubscript{r} (°C)</th>
<th>T\textsubscript{m} (°C)</th>
<th>P\textsubscript{m} (g/cm\textsuperscript{3})</th>
<th>k\textsubscript{m}</th>
<th>Δk\textsubscript{m} x 10\textsuperscript{5} (F-C)</th>
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These results show that the polynominal fitting procedure is less accurate in predicting the nonlinear dependance of the cross sections on moderator density. We can also draw some other conclusions from this analysis. The cross sections dependance on moderator density is the strongest and care should be taken when using density as a feedback parameter.

### 3.2 Summary

This chapter presented an initial investigation into the dependence of cross sections on thermal-hydraulic feedback parameters. This analysis used existing methodologies to show that with the existing cross section libraries, the moderator density affects the neutron flux more than any other feedback parameter. This chapter also demonstrated the nonlinear behavior of the cross sections dependencies on the thermal-hydraulic feedback parameters.
Chapter 4

THE COUPLING TERMS AND MATRIX SOLUTION

4.1 Formulation of the Non-Linear Coupling Terms

In the previous chapters we have developed a clear research path and demonstrated the need to improve the temporal coupling between TRACE/PARCS. The current state-of-the-art research has shown some promise but has not been adapted to full scale reactor analysis codes. The methods that have tried to approximate implicit temporal coupling for reactor analysis codes have had less than favorable results. The deficiencies of these attempts can be overcome if the proper care is used in the formulation of a complete set of consistent equations. This chapter presents the basic mathematical model, which will be used to address the problems associated with the current methods.

The details of the fluid/temperature and neutron balance equations are presented in Chapter 2. This chapter will concentrate on the details of the coupling terms and the proposed solution technique. With any set of equations that is to be solved each equation will have a number of unknowns and it is desirable to reduce the number of unknowns to as few as possible. The key here is to formulate the current equations into a complete consistent set which can be solved as one large system. From the fluid dynamics field equations we obtain the following unknowns $P, P_a, T_f, T_g, \alpha, (V_l, V_g)$; From the heat conduction we have the heat structure temperatures, $T_f$, as the only unknown, and from the neutronics equations we have $\phi_1, \phi_2, (C_l)$ where $l = 1, 6$ as the unknowns. There are 16 unknowns all together so that means we need a total of 16 equations. The 16 equations consist of the 6 two-phase flow equations plus the non-condensable mass equation, one heat conduction equation, the two-group neutron diffusion equation, and the 6 precursor equations. In
practical reactor physics and thermal hydraulic calculations these variables are not all unknowns. In TRACE the liquid and gas velocity are a linear function of the cell center pressure. The precursor density concentrations are assumed to be functions of the old time flux. This brings our set of unknowns down to 8. The coupling terms are the power sent to the heat conduction equation and the total pressure, partial pressure of non condensable gas, liquid temperature, and vapor temperature. In the neutron balance equation the cross sections are dependant on these thermal-hydraulic feedback parameters.

The semi-implicit form of the gas and mixture energy equations (2-32) and (2-33) is shown in equations (4-1) and (4-2). The energy equations are given here:

**Gas Energy:**

\[
\begin{align*}
\left[ \alpha^+ \frac{n+1}{\rho_g^n e_g^n} - \alpha^n \rho_g^n e_g^n \right] \frac{n}{\Delta t} + \nabla \cdot \left( \alpha^n \rho_g^n e_g^n V_g^n \right) = \\
-P^n \left[ \frac{(\alpha^+ - \alpha^n)}{\Delta t} + \nabla \cdot \left( \alpha^n V_g^n \right) \right] + \Gamma^n h_{fg} \rho_{w} + q_{wg} + q_{ig} + q_{dg}
\end{align*}
\] (4-1)

**Mixture Energy:**

\[
\begin{align*}
\left[ \alpha^+ \frac{n+1}{\rho_g^n e_g^n} + (1 - \alpha^+) \rho_l^n e_l^n - \alpha^n \rho_g^n e_g^n - (1 - \alpha^n) \rho_l^n e_l^n \right] \frac{n}{\Delta t} + \nabla \cdot \left( \alpha^n \rho_g^n e_g^n V_g^{n+1} \right) + P^n \nabla \cdot \left[ \alpha^n V_g^n + (1 - \alpha^n) V_l^{n+1} \right] = \\
q_{wg} + q_{wl} + q_{ig} + q_{dg}
\end{align*}
\] (4-2)
Where:

\[ q_{wg}^{n+1} = h_{wg}^n a_w (T_{w}^{n+1} - T_g^n) \]  
(4-3)

\[ q_{wl}^{n+1} = h_{wl}^n a_w (T_{w}^{n+1} - T_l^n) \]  
(4-4)

The important terms here are the new time energy deposited in the gas and liquid phases. These are the term coupling the heat conduction equations to the fluid equations through the new time wall temperature term \( T_w^{n+1} \). The wall temperature is calculated by the heat conduction equation shown in equation (4-5).

\[
\begin{align*}
(\rho c_p)_{ij} T_{ij}^{n+1} - T_{ij}^n &= \frac{1}{2} \left[ r_i \Delta r_i + \frac{\Delta r_i^2}{4} \right] + \left( r_i \Delta r_{i-1} - \frac{\Delta r_{i-1}^2}{4} \right) \left[ \frac{\Delta z_j + \Delta z_{j-1}}{2} \right] \\
&= \left\{ r_{i+1/2} k_{i+1/2,j} \left( T_{i+1,j}^{n+1} - T_{ij}^{n+1} \right) / \Delta r_i + r_{i-1/2} k_{i-1/2,j} \left( T_{i-1,j}^{n+1} - T_{ij}^{n+1} \right) / \Delta r_{i-1} \right\} \\
&\times \left[ \frac{\Delta z_j + \Delta z_{j-1}}{2} \right] + \left\{ k_{i,j+1/2} \left( T_{i,j+1}^n - T_{ij}^n \right) / \Delta z_j + k_{i,j-1/2} \left( T_{i,j-1}^n - T_{ij}^n \right) / \Delta z_{j-1} \right\} \\
&\times \frac{1}{2} \left[ r_i \Delta r_i + \frac{\Delta r_i^2}{4} \right] + \left( r_i \Delta r_{i-1} - \frac{\Delta r_{i-1}^2}{4} \right)
\end{align*}
\]  
(4-5)

The energy deposited in the fluid \( q_{wg}^{n+1} \) and \( q_{wl}^{n+1} \) are boundary conditions on equation (4-5). The heat conduction equation requires the volumetric heat generation rate \( q''^{m+1} \). This is obtained from the local flux using equation (4-6).
\[ q_f = \gamma_k \sum_{g=1}^{G} \xi_g \phi_g \]  

(4-6)

Where \( \gamma \) is the fraction of power deposited into the fuel and is defined as \( \gamma = 1 - \gamma \).

The new time formulation for equation (4-6) for two energy groups is:

\[ q_{f}^{n+1} = \gamma_k \left[ (f_1 + \phi_1^{n+1}) + (f_2 + \phi_2^{n+1}) \right] \]  

(4-7)

The new time fluxes are determined using the coarse mesh finite difference form of the nodal balance equation. However, the cross sections have to be formulated in terms of the new time total pressure, non-condensable pressure, fuel temperature, liquid temperature, vapor temperature and void fraction. The first step is to formulate the cross sections in terms of these feedback parameters. For any generic cross section \( x \) for each group we can expand the cross section and write it as a function of fuel temperature and density as shown in equation (4-8).

\[ \Sigma_x(T_f, \rho_m) = \Sigma_x(T_f^r, \rho_m^r) + (T_f - T_f^r) \frac{\partial \Sigma_x}{\partial T_f} + (\rho_m - \rho_m^r) \frac{\partial \Sigma_x}{\partial \rho_m} \]  

(4-8)

The superscript \( r \) in equation (4-8) indicates a reference thermal-hydraulic parameter. The TMI MSLB and the PB TT benchmark problems with will be used in this analysis both used tabulated cross sections based on fuel temperature and density. The derivatives of the cross sections with respect to fuel temperature and density are not tabulated as in the polynomial fitting procedure so they will be calculated by linear interpolation of the total cross sections tabulated in the libraries. Therefore it is necessary to write the density dependence as a function of total pressure, partial pressure of noncondensable gas, liquid temperature, gas temperature and void fraction. In a similar manner to the above expansion the density derivative can be rewritten as shown in equation (4-9)
The derivatives of the density with respect to the individual thermal hydraulic parameters are calculated by the TRACE thermodynamic properties routines and thus are known quantities. The partial derivatives of the density in equation (4-9) are obtained from the equation of state in TRACE using the following mixture density definition:

\[ \rho_m = \alpha \rho_a(P_a, T_g) + \alpha \rho_g(P, T_g) + (1 - \alpha) \rho_l(P, T_l) \]

The partial derivative of the mixture density with respect to each of the thermal hydraulic feedback parameter is:

\[ \frac{\partial \rho_m}{\partial P} = \alpha \frac{\partial \rho_g}{\partial P} + (1 - \alpha) \frac{\partial \rho_l}{\partial P} \]

\[ \frac{\partial \rho_m}{\partial T_g} = \alpha \frac{\partial \rho_a}{\partial T_g} + \alpha \frac{\partial \rho_g}{\partial T_g} \]

\[ \frac{\partial \rho_m}{\partial P_a} = \alpha \frac{\partial \rho_a}{\partial P_a} \]

\[ \frac{\partial \rho_m}{\partial T_l} = (1 - \alpha) \frac{\partial \rho_l}{\partial T_l} \]

The change in the individual parameter from a reference point (i.e. \( T_f = T_f^r = \delta T_f \)) is now consistent with those unknowns found in the fluid and heat conduction equations. The new time cross sections are then given by equation (4-10).
At this point it is important to note that the rest of this derivation assumes that the last best guess at the current cross section \( \Sigma_x^{n+1} \) is equal to the old time cross section \( \Sigma_x^n \). This means that we are assuming that the time step is small enough that the difference in the cross section within a time step can be accounted by using the first order expansion terms in Equation (4-10).

\[
\Sigma_x^{n+1} = \Sigma_x^{n+1(k)} + \delta \Sigma_x = \Sigma_x^n + \delta T_f \left( \frac{\partial \Sigma_x}{\partial T_f} \right)^n
\]

\[
+ \left[ \delta T_g \left( \frac{\partial \rho_m}{\partial T_g} \right)^{(k)} + \delta T_l \left( \frac{\partial \rho_m}{\partial T_l} \right)^{(k)} + \delta P_a \left( \frac{\partial \rho_m}{\partial P_a} \right)^{(k)} + \delta P \left( \frac{\partial \rho_m}{\partial P} \right)^{(k)} + \delta \alpha \left( \frac{\partial \rho_m}{\partial \alpha} \right)^{(k)} \right] \partial \Sigma_x \frac{\partial \rho_m}{\partial \rho_m}
\]

At this point it is important to note that the rest of this derivation assumes that the last best guess at the current cross section \( \Sigma_x^{n+1(k)} \) is equal to the old time cross section \( \Sigma_x^n \). This means that we are assuming that the time step is small enough that the difference in the cross section within a time step can be accounted by using the first order expansion terms in Equation (4-10).

At this point we have enough pieces to construct a consistent set of thermal-hydraulic, heat transfer, and neutronic equations. The coupling terms in these equations are all based on new time power and thermal-hydraulic feedback parameters. This formulation is now fully implicit in the time for the coupling terms between the thermal hydraulics, heat conduction, and neutronics. Since the new time power deposited in the fuel is dependant on the new time flux that is in turn dependant on the new time thermal-hydraulic feedback parameters which are dependent on the power deposited in the fuel, the system of equations developed in this section are nonlinear and require special techniques to solve these systems. The solution to these equations are discussed later in this thesis. The next section details the linearized system of equations based on these implicit coupling terms formulated in this section.

### 4.2 Coupling Coefficients

Based on the equations discussed in section 4.1 the Matrix coefficients can be developed. This section is a detailed look at those coefficients. I will present the Semi-Implicit form for each of the mass and energy equations and then develop the linearized form for the coupling coefficients for each term of interest in this thesis.
4.2.1 Mixture Energy Equation

To develop the linearized form of the mixture energy equation we need to start with Equation (2-46). Move the heat rate to the left hand side of the equation. At this point we are concerned with the heat rate from the wall to the gas phase and the liquid phase. To make these terms consistent with the linearized formulation of the energy equation we use a simple first order approximation. This states that our new time feedback parameter is equal to the last best guess at the new time value plus a small change in the value. For simplicity the new time iterate \((n+1(k))\) will be written as \((k)\) only.

\[
\begin{align*}
\alpha_j^{n+1} &- \rho g_j^{n+1} e_{gj}^{n+1} + (1 - \alpha_j^{n+1}) \rho l_j^{n+1} e_{lj}^{n+1} - \alpha_j^n \rho g_j^n e_{gj}^n - (1 - \alpha_j^n) \rho l_j^n e_{lj}^n \\
\Delta t \\
\n+ \nabla_j \cdot \left[ \alpha^n \rho g^n e_g^n \dot{V}_g^{n+1} + (1 - \alpha^n) \rho_j^n e_j^n \dot{V}_l^{n+1} \right] \\
+ \rho_l^n \nabla_j \cdot \left[ \alpha^n \dot{V}_g^{n+1} + (1 - \alpha^n) \dot{V}_l^{n+1} \right] \\
- q_{wg}^{n+1} - q_{wl}^{n+1} = q_{dl}^n + q_{dg}^n
\end{align*}
\]

At this point we are concerned with the heat rate from the wall to the gas phase and the liquid phase. To make these terms consistent with the linearized formulation of the energy equation we use a simple first order approximation \(U^{n+1} = U^{n+1(k)} + \delta U\). This states that our new time feedback parameter is equal to the last best guess at the new time value plus a small change in the value. For simplicity the new time iterate \((n+1(k))\) will be written as \((k)\) only.

\[
\begin{align*}
q_{wg}^{n+1} &= h_{wg}^n a_w (T_w^{(k)} + \delta T_w - T_g^{(k)} - \delta T_g) \quad (4-11) \\
q_{wl}^{n+1} &= h_{wl}^n a_w (T_w^{(k)} + \delta T_w - T_l^{(k)} - \delta T_l) \quad (4-12)
\end{align*}
\]

The heat rates shown in Equations (4-11) and (4-12) are defined in terms of the last guess at the wall, gas, and liquid temperature plus a small change in these temperatures. The perturbed temperature now becomes the unknowns in Equations (4-11) and (4-12). With the heat rates redefined we can now write the linearized mixture equation as:
The coefficients highlighted in red in Equation (4-13) are added to the liquid and vapor terms in the overall matrix. A new unknown is also added to the mixture energy equation to account for the wall temperature terms. Finally the last guess at the new time heat rates are moved to the right hand side of Equation (4-13). This increases the number of unknowns in the mixture energy equation for each thermal hydraulic finite volume to six unknowns.

\[
\left[ \frac{\partial (\alpha \rho ve_v)}{\partial \alpha} \right] Vol_v + \left[ \frac{\partial ((1-\alpha)\rho ve_l)}{\partial \alpha} \right] Vol_l - \alpha \rho ve_ve_v A \Delta t - (1-\alpha) \rho ve_l V e l A \Delta t \right] \delta P (4-13)
\]

\[
+ \left[ \frac{\partial (\alpha \rho ve_v)}{\partial \alpha} \right] Vol_v + \left[ \frac{\partial ((1-\alpha)\rho ve_l)}{\partial \alpha} \right] Vol_l \delta \alpha
\]

\[
+ \left[ \frac{\partial (\alpha \rho ve_v)}{\partial T_v} \right] Vol_v - (-h_{wg}^n a_w) \Delta t \right] \delta T_v
\]

\[
+ \left[ \frac{\partial ((1-\alpha)\rho ve_l)}{\partial T_l} \right] Vol_l - (-h_{wl}^n a_l) \Delta t \right] \delta T_l
\]

\[
+ \left[ \frac{\partial (\alpha \rho ve_a)}{\partial P_a} \right] Vol_v \delta P_a
\]

\[
+ [- h_{wg}^n a_w \Delta t - h_{wl}^n a_l \Delta t] \delta T_w
\]

\[
= [\alpha \rho ve_v - \alpha \rho ge_v] Vol_v + \alpha \rho ve_ve_v A \Delta t + \alpha \rho ve_e PA \Delta t
\]

\[
+ [(1-\alpha)\rho ve_l - (1-\alpha)\rho ve_l] Vol_l + (1-\alpha)\rho ve_l V e l A \Delta t + (1-\alpha) \rho ve_l PA \Delta t
\]

\[
+ \left[ h_{wg}^n a_w T_w^{(k)} - h_{wg}^n a_w T_g^{(k)} + h_{wl}^n a_w T_w^{(k)} - h_{wl}^n a_w T_l^{(k)} \right] \Delta t
\]

The coefficients highlighted in red in Equation (4-13) are added to the liquid and vapor terms in the overall matrix. A new unknown is also added to the mixture energy equation to account for the wall temperature terms. Finally the last guess at the new time heat rates are moved to the right hand side of Equation (4-13). This increases the number of unknowns in the mixture energy equation for each thermal hydraulic finite volume to six unknowns.
4.2.2 Gas Energy Equation

Similar arguments can be made for the gas energy equation as for the mixture energy equation (2-45).

\[
\frac{[\alpha_j^{n+1} \rho_{gi}^{n+1} e_{gi}^{n+1} - \alpha_j^n \rho_{gi}^n e_{gi}^n]}{\Delta t} + \nabla \cdot (\alpha_j^n \rho_{gi}^n e_{gi}^n \mathbf{v}_g^{n+1}) \\
+ p^{n+1} \left[ \frac{(\alpha_j^{n+1} - \alpha_j^n)}{\Delta t} + \nabla \cdot (\alpha_j^n \mathbf{v}_g^{n+1}) \right] - q_{wg}^{n+1} = \Gamma_{fg}^{n+1} + q_{ig}^n + q_{dg}^n
\]

As in the mixture energy equation, the definition of the heat rate to the gas phase is given in Equation (4-11). Plugging Equation (4-11) into the gas energy equation linearized gas equation is given in Equation (4-14).

\[
\alpha \left[ \frac{\partial e_v}{\partial P_v} + e_v \frac{\partial \rho_v}{\partial P_v} \right] Vol_v - \alpha V \nu \Delta t - \alpha Vol \right] \delta P
\]

\[
\left[ \left( \frac{\partial (\alpha \rho_v e_v)}{\partial \alpha} \right) Vol_v + PVol \right] \delta \alpha + \left[ \left( \frac{\partial (\alpha \rho_v e_v)}{\partial T_v} \right) Vol_v - (-h_{wg}^n a_w) \Delta t \right] \delta T_v
\]

\[
+ \left[ \left( \frac{\partial (\alpha \rho_a e_a)}{\partial P_a} \right) Vol_v \right] \delta P_a + \left[ -h_{wg}^n a_w \Delta t \right] \delta T_w
\]

\[
= [\alpha \rho_v e_v - \alpha \rho_{gi} e_{gi}] Vol_v + \alpha \rho_v V \nu e_v \Delta t + \alpha V \nu P \Delta t + \alpha PVol
\]

\[
+ \left[ h_{wg}^n a_w T_w^{(k)} - h_{wg}^n a_w T_g^{(k)} \right] \Delta t
\]

As in the mixture energy equation the new terms are shown in red.

4.2.3 Mass Equation
The mass equation contains a term for the vapor generation rate when the bulk fluid temperature is subcooled but nucleate boiling occurs next to the wall. The term $\Gamma_{\text{sub}}$ is calculated as follows:

$$\Gamma_{\text{sub}} = \frac{f_{\text{sub}} \cdot h_{\text{wl}} \cdot (T_w - T_l) \cdot A''_{\text{w}}}{h_{\text{fg}}} \quad (4-15)$$

**Gas Mass**

$$\frac{\alpha_j^{n+1} \rho_g^{n+1} - \alpha_j^n \rho_g^n}{\Delta t} + \nabla_j \cdot [\alpha_g^n \rho_g^n T_l^{n+1}] = \Gamma_i^{n+1} + \Gamma_{\text{sub}}^{n+1}$$

At this point we are concerned with the heat rate from the wall to the gas phase. To make these terms consistent with the linearized formulation of the gas mass equation.

$$\Gamma_{\text{sub}} = \frac{f_{\text{sub}} \cdot h_{\text{wl}}^n \cdot (T_w^{n+1(k)} + \delta T_w - T_l^{n+1(k)} - \delta T_l) \cdot A''_{\text{w}}}{h_{\text{fg}}^n} \quad (4-16)$$

The following coefficients are then added to the liquid terms in the overall matrix:

$$\frac{f_{\text{sub}} \cdot h_{\text{wl}}^n \cdot A''_{\text{w}}}{h_{\text{fg}}^n} \text{ for each } \delta T_{ij} \text{ unknown.}$$

The following off diagonal terms are added to the gas mass equations.

$$\frac{f_{\text{sub}} \cdot h_{\text{wl}}^n \cdot A''_{\text{w}}}{h_{\text{fg}}^n} \text{ for each } T_{wj}^{n+1}$$

The following terms have to be added to the right hand side of the gas energy equation.
\[
\frac{f_{sub} \cdot h_{wl}^n \cdot A_w^m}{\dot{h}_{fg}^n} T_l^n
\]

**Liquid Mass**

\[
\frac{(1 - \alpha_j^{n+1}) \rho_{lj}^{n+1} - (1 - \alpha_j^n) \rho_{lj}^n}{\Delta t} + \nabla_j \cdot \left[ (1 - \alpha^n) \rho_j^n V_i^{n+1} \right] = -\Gamma_i^n + \Gamma_{sub}^{n+1}
\]

The term here in the liquid mass equation is the same as that in the gas mass equation just with an opposite sign. The following coefficients are then added to the liquid terms in the overall matrix:

\[
\frac{f_{sub} \cdot h_{wl}^n \cdot A_w^m}{\dot{h}_{fg}^n} \text{ for each } \delta T_{ij} \text{ unknown.}
\]

The following off diagonal terms are added to the gas mass equations.

\[
\frac{f_{sub} \cdot h_{wl}^n \cdot A_w^m}{\dot{h}_{fg}^n} \text{ for each } T_{wj}^{n+1}
\]

The following terms have to be added to the right hand side of the gas energy equation.

\[
\frac{f_{sub} \cdot h_{wl}^n \cdot A_w^m}{\dot{h}_{fg}^n} \text{ for each } T_l^{n}
\]

**4.2.4 Heat Conduction Equation**
The liquid and vapor temperatures enter the heat conduction equation through the boundary conditions. For the inner surface of the wall the heat conduction equation (2-53) can be written as:

\[
-\left(\frac{r_{3/2}k_{3/2}}{\Delta r_1} + \frac{1}{2} \left( r_1 \Delta r_1 + \frac{\Delta r_1^2}{4} \right) \left( \frac{\rho C_p}{\Delta t} \frac{3/2}{r_1} + r_1 (h_l + h_g) \right) T_1^{n+1} + \frac{r_{3/2}k_{3/2}}{\Delta r_1} T_2^{n+1}\right) (4-17)
\]

\[
= -\frac{1}{2} \left( r_1 \Delta r_1 + \frac{\Delta r_1^2}{4} \right) \left[ \left( \frac{\rho C_p}{\Delta t} \frac{3/2}{r_1} + q'''_{n+1} \right) - r_1 [h_l T_l^{n+1} + h_g T_g^{n+1}] \right]
\]

Equation (4-17) is a special case of the generalized heat conduction equation. It is presented here to show where the liquid and gas temperatures come into the heat conduction equation. The rest of the discussion in this section will concentrate on the generalized form of the heat conduction equation. The liquid and gas temperatures in equation (4-17) are perturbed in the same manner as all other variables in this Thesis. They will not be explicitly shown in the following derivation but are accounted for in the final matrix. Pulling the power deposited in the fuel out of the right hand side, the generalized form of Equation (2-53) can be written as:

\[
a_{1,i,j} T_i^{n+1} - a_{2,i,j} T_{i+1,j}^{n+1} - a_{3,i,j} T_{i-1,j}^{n+1} = b_{i,j} + q'''_{n+1} (4-18)
\]

For the generalized form the coefficients are defined as:

\[
a_{2,i,j} = \frac{(\rho C_p)_{i,j}}{\Delta t} + \frac{r_{i+1/2}k_{i+1/2,j}}{\Delta r_i \Delta r_j} + \frac{r_{i-1/2}k_{i-1/2,j}}{\Delta r_i \Delta r_{i-1}} (4-19)
\]

\[
a_{3,i,j} = \frac{r_{i+1/2}k_{i+1/2,j}}{\Delta r_i \Delta r_j} (4-20)
\]
\[ a_{1,i,j} = \frac{r_{i-\frac{1}{2}}k_{i-\frac{1}{2},j}}{\rho_i \Delta r_{i-1}} \]  

\[ b_{i,j} = \left( \frac{(\rho C_p)_{i,j}}{\Delta t} - \frac{k_{i,j+\frac{1}{2}}}{\varepsilon_j \Delta z_j} - \frac{k_{i,j-\frac{1}{2}}}{\varepsilon_j \Delta z_{j-1}} \right) \frac{T^n_{i,j}}{\varepsilon_j \Delta z_j} + \frac{k_{i,j+\frac{1}{2}}}{\varepsilon_j \Delta z_j} T^n_{i,j+1} + \frac{k_{i,j-\frac{1}{2}}}{\varepsilon_j \Delta z_{j-1}} T^n_{i,j-1} \]  

The power deposited in the fuel is then given by:

\[ q^{n+1}_{i,j} = \tilde{\gamma} \kappa \sum_{f=1}^{n+1} \phi_1^{n+1} + \tilde{\gamma} \kappa \sum_{f=2}^{n+1} \phi_2^{n+1} \]  

Equation (4-23) is dependent on both the fission cross section and the fast and thermal flux. The fast and thermal flux are unknowns and the fission cross sections are dependent on the thermal hydraulic variables. This means that the power deposited in the fuel has to be linearized. This is done in a consistent manner to the thermal hydraulic equations.

\[ q^{n+1}_{i,j} = \tilde{\gamma} \kappa (\sum_{f=1}^{n+1} \phi_1^{n+1} + \delta \Sigma_{f=1}) (\phi_1^{n+1} + \delta \phi_1) + \tilde{\gamma} \kappa (\sum_{f=2}^{n+1} \phi_2^{n+1} + \delta \Sigma_{f=2}) (\phi_2^{n+1} + \delta \phi_2) \]  

Multiplying through and discarding all of the higher order terms, Equation (4-24) becomes:

\[ q^{n+1}_{i,j} = \tilde{\gamma} \kappa \sum_{f=1}^{n+1} \phi_1^{n+1} + \tilde{\gamma} \kappa \sum_{f=1}^{n+1} \phi_1^{n+1} \delta \Sigma_{f=1} + \tilde{\gamma} \kappa \sum_{f=2}^{n+1} \phi_2^{n+1} + \tilde{\gamma} \kappa \sum_{f=2}^{n+1} \phi_2^{n+1} \delta \Sigma_{f=2} \]  

Using these definitions as well as \( T^{n+1} = T^{n+1}(k) + \delta T \) and placing these into Equation (4-18) a new linearized form for the heat conduction is shown in equation (4-26).
At this point it is necessary to expand the cross sections in terms of the unknown variables. Using Equation (4-11) the linearized residual heat conduction equation is given in equation (4-27).

\[
a_{2, i, j}(\delta T_{i, j}) - a_{3, i, j}(\delta T_{i+1, j}) - a_{1, i, j}(\delta T_{i-1, j}) = b_{i, j} - a_{2, i, j}T_{i, j}^{n+1(k)} + a_{3, i, j}T_{i+1, j}^{n+1(k)} + a_{1, i, j}T_{i-1, j}^{n+1(k)}
\]

\[+ \gamma \kappa \Sigma_{f1}^{n+1(k)} \phi_{1} + \gamma \kappa \Sigma_{f2}^{n+1(k)} \phi_{2} + \gamma \kappa \Sigma_{f1}^{n+1(k)} \phi_{1} + \gamma \kappa \Sigma_{f2}^{n+1(k)} \phi_{2}^{n+1(k)}
\]

\[= b_{i, j} - a_{2, i, j}T_{i, j}^{n+1(k)} + a_{3, i, j}T_{i+1, j}^{n+1(k)} + a_{1, i, j}T_{i-1, j}^{n+1(k)} + \gamma \kappa \Sigma_{f1}^{n} \phi_{1} + \gamma \kappa \Sigma_{f2}^{n} \phi_{2}
\]
As in the fluid equations the new terms are highlighted in red. However, in the heat conduction equation the old time temperature terms on the right hand side of this equation are also new since the current implementation of the heat conduction equation does not solve a residual equation it solves directly for the temperatures in the metal.

4.2.5 Neutronics Equations

The following section documents the derivation of the residual equations for the two-group finite difference formulation of the diffusion equation transient fixed source problem. This section is broken into two parts. The first part represents the fast group diffusion equation and the second part is the thermal group equation.

Fast Group Equation:

\[
\begin{align*}
\left( \Sigma_{r1} - \beta_p \lambda \Sigma_f \right) & \phi_1^{m,n+1} - \beta_p \lambda \Sigma_f \phi_2^{m,n+1} + L_1^{m,n+1} \\
= S_1^{m,n+1} + S_d^{m,n}
\end{align*}
\]

(4-28)

Where:

\[
\Sigma_{rg}^{m,n+1} = \frac{1}{\Theta v_g^m \Delta t_{n+1}} + \frac{\alpha_g^{m,n+1}}{v_g^m} + \Sigma_{rg}^{m,n+1}
\]

\[
S_g^{m,n+1} = \left[ \left( \frac{1}{\Theta v_g^m \Delta t_{n+1}} + \Theta \alpha_g^{m,n+1} \right) \phi_g^{m,n} + \Theta R_g^{m,n+1} \right] e^{\alpha_g^{m,n+1} \Delta t_{n+1}}
\]

\[
\tilde{S}_d^n = \sum_{k=1}^{K} \kappa_k \tilde{\lambda}_k C_k^n + \sum_{l=n-1}^{n} \sum_{k=1}^{K} \beta_k \Omega_k^l \Psi_k
\]
The notation used here is consistent with that used in the PARCS manual. For a more complete description of individual terms see reference [24]. In the original formulation of the finite difference formulation of the diffusion equation the cross sections are all known values. In this formulation the cross sections contain unknowns. Equation (4-28) has to be linearized. Assume that the cross sections and flux terms can be written as follows:

Let: \( \Sigma_x^{m,n+1} = \Sigma_x^{m,(k)} + \delta \Sigma_x^{m} \) and \( \phi_g^{m,n+1} = \phi_g^{m,(k)} + \delta \phi_g^{m} \)

The node superscript Placing these into equation (4-28) multiply through and remove higher order terms, Equation (4-28) becomes:

\[
\tilde{\Sigma}_1^{m,(k)} + \tilde{\phi}_1^{m,(k)} + \tilde{\phi}_1 = \tilde{\Sigma}_1^{m,(k)} + \tilde{\phi}_1^{m,(k)} - \beta_p^{m,(k)} \lambda \phi_1^{m,(k)} \delta \phi_1^{m} - \beta_p^{m,(k)} \lambda \phi_1^{m,(k)} \phi_1^{m,(k)} \\
- \beta_p^{m,(k)} \lambda \phi_2^{m,(k)} \delta \phi_2^{m} - \beta_p^{m,(k)} \lambda \phi_2^{m,(k)} \phi_2^{m,(k)} \\
- \beta_p^{m,(k)} \lambda \phi_2^{m,(k)} \phi_2^{m,(k)} + L_1^{n+1} = S_1^{(k)} + \tilde{s}_d^n
\]

Equation (4-30) shows the Coefficients for all 8 unknowns in this equation. Not shown in Equation 6 is the leakage coefficients. An additional term is added to equation (4-30) to account for the weighting of the fuel temperature. This weighting factor accounts for more than one fuel region being present in the heat conduction model. A average fuel temperature is used as the Doppler temperature used to calculate the cross sections. This average temperature is calculated using the volume weighting of the individual heat conduction regions in the fuel region. The weighting factor shown in equation (4-30) is calculated using:

\[
w_i = \frac{V_i}{V_{Total}} \quad \text{Where:} \quad V_i \text{ is the volume of an individual heat conduction node} \\
\]

\[V_{Total} \text{ is the total volume of the fuel region.}\]
For simplicity the following more compact notation will be used in subsequent equations.

\[
\begin{align*}
    &= S_1^n + S_d^n - \Sigma r_1 \phi_1 + \beta_p \nabla S_{f1} \phi_2 - \beta_p \nabla S_{f2} \phi_1 - \beta_p \nabla \phi_1 - \beta_p \nabla \phi_2
\end{align*}
\]

\[
\frac{\partial \delta M_1}{\partial U} \delta U = \left[ \phi_1^{m,k} \left( \frac{\partial \Sigma_{r1}}{\partial \rho_m} - \beta_p \nabla \frac{\partial \Sigma_{f1}}{\partial \rho_m} \right) + \phi_2^{m,k} \left( \beta_p \nabla \frac{\partial \Sigma_{f2}}{\partial \rho_m} \right) \right] \left( \frac{\partial \rho_m}{\partial U} \right)^{(k)} \delta U
\]

where: \( U = P, \alpha, T_g, T_r, P_a \)
The leakage terms for both the fast and thermal group equations is shown in Equation (4-31). Equation (4-31) shows the leakage terms for time step n+1 for node m. u represents the direction (i.e x,y,z). The problem lies in the coefficients \( a_{gu}^m, a_{gu}^m, \) and \( a_{gu}^m \). As shown in Equation (4-31) these coefficients are represented by a first order estimate of the nodal coupling based on the finite difference approximation, which represents the nodal coupling coefficients as a combination of diffusion coefficients for the current cell and neighboring node. This causes a problem with the linearization.

\[
L_{gu}^m = a_{gu}^m \phi_g^m + a_{gu}^m \phi_g^m + a_{gu}^m \phi_g^m
\]  

(4-31)

Let the linearized leakage term be defined as:

\[
L_{gu}^{m,n+1} = L_{gu}^{m,k} + \delta L_{gu}^m + \frac{\partial \delta L_{gu}^m}{\partial P} \delta P + \frac{\partial \delta L_{gu}^m}{\partial \alpha} \delta \alpha + \frac{\partial \delta L_{gu}^m}{\partial T_g} \delta T_g
\]

\[
+ \frac{\partial \delta L_{gu}^m}{\partial T_l} \delta T_l + \frac{\partial \delta L_{gu}^m}{\partial P_a} \delta P_a + \frac{\partial \delta L_{gu}^m}{\partial T_f} \delta T_f
\]  

(4-32)

Then let:

\[
L_{gu}^{m,k} = [a_{gu}^m]^n \phi_g^m + [a_{gu}^m]^n \phi_g^m + [a_{gu}^m]^n \phi_g^m
\]

\[
\delta L_{gu}^m = [a_{gu}^m]^n \delta \phi_g + [a_{gu}^m]^n \delta \phi_g + [a_{gu}^m]^n \delta \phi_g
\]

\[
\frac{\partial \delta L_{gu}^m}{\partial U} \delta U = \left( [\phi_g^m]^n \frac{\partial \delta a_{gu}^m}{\partial U} + [\phi_g^m]^n \frac{\partial \delta a_{gu}^m}{\partial U} + [\phi_g^m]^n \frac{\partial \delta a_{gu}^m}{\partial U} \right) \delta U
\]
The leakage term for each x,y,z direction is given as:

\[
L_{gu}^{m,n+1} = \left[ a_{gu}^m \right]^{n} \phi_g^m + \left[ a_{gu}^m \right]^n \phi_g^m + \left[ a_{gu}^m \right]^n \phi_g^m + \left[ \frac{\partial a_{gu}^m}{\partial \alpha} \right]^n \phi_g + \left[ \frac{\partial a_{gu}^m}{\partial T_g} \right]^n \phi_g + \left[ \frac{\partial a_{gu}^m}{\partial T_l} \right]^n \phi_g + \left[ \frac{\partial a_{gu}^m}{\partial P_a} \right]^n \phi_g + \left[ \frac{\partial a_{gu}^m}{\partial T_f} \right]^n \phi_g
\]

In equation (4-33) the derivative of the leakage coefficients is given. These coefficients are determined by averaging the diffusion coefficients between nodes to estimate a cell edge diffusion coefficient for each edge.

NOTE: PARCS also includes a corrective nodal coupling coefficient. This coefficient is assumed to be zero for this application.

\[
a_{gu}^m = \frac{1}{h_u^m} \tilde{D}_{gu}^m
\]  

where: \( U = P, \alpha, T_g, T_l, P_a, T_f \)
Equation (4-37) shows the current method for calculating the coupling coefficient. The diffusion coefficients in this equation have the same dependencies as the cross sections on the thermal hydraulic and heat conduction parameters. To simplify this equation’s dependency on these parameters, equation (4-38) shows the simplified representation of the perturbed nodal coupling coefficient.

\[
a_{gu}^m = \frac{1}{h_u^m} \left( \tilde{D}_{gu}^{m+} + \tilde{D}_{gu}^{m-} \right)
\]

\[
a_{gu}^{m+} = -\frac{1}{h_u^m} \tilde{D}_{gu}^{m+}
\]

Equation (4-37) shows the current method for calculating the coupling coefficient. The diffusion coefficients in this equation have the same dependencies as the cross sections on the thermal hydraulic and heat conduction parameters. To simplify this equation’s dependency on these parameters, equation (4-38) shows the simplified representation of the perturbed nodal coupling coefficient.

\[
\tilde{D}_{gu}^{m\pm} = \frac{2D_g^{m\pm} D_g^m}{D_g^m \Delta u_m + D_g^m \Delta u_m^{\pm}}
\]

\[
\tilde{D}_{gu}^{n+1} = \tilde{D}_{gu}^{n} + \delta \tilde{D}_{gu} = \left[ \frac{2D_g^{m\pm} D_g^m}{D_g^m \Delta u_m + D_g^m \Delta u_m^{\pm}} \right]^n + \delta \tilde{D}_{gu}
\]

The simplification that is applied to the coupling coefficient is the perturbed coefficient will be represented as a simple average of the diffusion coefficients for the adjoining cells. The leakage term is then linearized in the same manner as the rest of the terms.

\[
\tilde{D}_{gu}^{n+1} = \tilde{D}_{gu}^{n} + \delta \tilde{D}_{gu} = \left[ \frac{2D_g^{m\pm} D_g^m}{D_g^m \Delta u_m + D_g^m \Delta u_m^{\pm}} \right]^n + \frac{\delta D_g^m}{2} + \delta \tilde{D}_{gu}
\]

The change in the diffusion coefficient for the current cell and the adjacent cells can be represented using the same expansion as before. The expansions are shown in equations (4-40) and (4-41).
\[
\frac{\delta D_g^{m \pm}}{2} = \frac{1}{2} \left[ \delta T_f \frac{\partial D_g^{m \pm}}{\partial T_f} + \delta T_g \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial \rho_m} + \delta T_l \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial \rho_m} \\
+ \delta P \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial P} + \delta \alpha \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial \alpha} \right] 
\]

(4-40)

\[
\frac{\delta D_g^{m}}{2} = \frac{1}{2} \left[ \delta T_f \frac{\partial D_g^{m}}{\partial T_f} + \delta T_g \frac{\partial \rho_m \partial D_g^{m}}{\partial \rho_m} + \delta T_l \frac{\partial \rho_m \partial D_g^{m}}{\partial \rho_m} + \delta P \frac{\partial \rho_m \partial D_g^{m}}{\partial P} + \delta \alpha \frac{\partial \rho_m \partial D_g^{m}}{\partial \alpha} \right] 
\]

(4-41)

Placing these expansions back into equation (4-34) and (4-36) the leakage coefficient for the neighboring nodes is shown in equation (4-42).

\[
\left[ a_g^{m \pm} \right]^{n + 1} = \frac{1}{h_u^m} \left[ \frac{2D_g^{m \pm} D_g^{m}}{D_g^{m \pm} \Delta u_m + D_g^{m} \Delta u_m \pm} \right]^n \\
- \frac{1}{2h_u^m} \left[ \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial P} + \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial \rho_m} \right]^{n} \delta P - \frac{1}{2h_u^m} \left[ \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial \alpha} + \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial \rho_m} \right]^{n} \delta \alpha \\
- \frac{1}{2h_u^m} \left[ \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial T_g} + \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial \rho_m} \right]^{n} \delta T_g \\
- \frac{1}{2h_u^m} \left[ \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial T_l} + \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial \rho_m} \right]^{n} \delta T_l \\
- \frac{1}{2h_u^m} \left[ \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial P_a} + \frac{\partial \rho_m \partial D_g^{m \pm}}{\partial \rho_m} \right]^{n} \delta P_a - \frac{1}{2h_u^m} \left[ \frac{\partial D_g^{m \pm}}{\partial T_f} + \frac{\partial D_g^{m \pm}}{\partial T_f} \right]^{n} \delta T_f
\]

The leakage coefficient for the current node is given in equation (4-43).
Using these definitions and placing them into equation (4-30), the fast group transient fixed source problem becomes:
Thermal Group Equation:

The linearized form of the thermal group equation follows the same derivation as the fast group equation. An abbreviated derivation for thermal energy group is presented here.

\[
\sum_i w_i \left[ \frac{\partial \delta W_i}{\partial T_f} + \frac{\partial \delta L_{1x}^m}{\partial T_f} + \frac{\partial \delta L_{1y}^m}{\partial T_f} + \frac{\partial \delta L_{1z}^m}{\partial T_f} \right] \delta T_f
\]

\[
+ \left[ \frac{\partial \delta M_1}{\partial P} + \frac{\partial \delta L_{1x}^m}{\partial P} + \frac{\partial \delta L_{1y}^m}{\partial P} + \frac{\partial \delta L_{1z}^m}{\partial P} \right] \delta P
\]

\[
+ \left[ \frac{\partial \delta M_1}{\partial T_g} + \frac{\partial \delta L_{1x}^m}{\partial T_g} + \frac{\partial \delta L_{1y}^m}{\partial T_g} + \frac{\partial \delta L_{1z}^m}{\partial T_g} \right] \delta T_g
\]

\[
+ \left[ \frac{\partial \delta M_1}{\partial P_a} + \frac{\partial \delta L_{1x}^m}{\partial P_a} + \frac{\partial \delta L_{1y}^m}{\partial P_a} + \frac{\partial \delta L_{1z}^m}{\partial P_a} \right] \delta P_a
\]

\[
+ \left[ \Sigma_{r1}^{m,n} - \beta_p \lambda \nu \Sigma_{f1}^{m,n} + a_{1x}^{m,n} + a_{1y}^{m,n} + a_{1z}^{m,n} \right] \delta \phi_1^{m,n} - \beta_p \lambda \nu \Sigma_{f2}^{m,n} \delta \phi_2^{m,n}
\]

\[
+ \left[ a_{1x}^{m,n} \delta \phi_1^{m,n} + a_{1y}^{m,n} \delta \phi_1^{m,n} \right]
\]

\[
+ \left[ a_{1z}^{m,n} \delta \phi_1^{m,n} \right]
\]

\[
+ \left[ a_{1y}^{m,n} \delta \phi_1^{m,n} \right]
\]

\[
+ \left[ a_{1z}^{m,n} \delta \phi_1^{m,n} \right]
\]

\[
+ \left[ a_{1x}^{m,n} \delta \phi_1^{m,n} \right]
\]

\[
S_2 = S_1^{(k)} + \delta S_d - \Sigma_{r1}^{m,n} \phi_1^{m,n} - \beta_p \lambda \nu \Sigma_{f2}^{m,n} \phi_2^{m,n}
\]

Thermal Group Equation:

The linearized form of the thermal group equation follows the same derivation as the fast group equation. An abbreviated derivation for thermal energy group is presented here.

\[
- \Sigma_{12}^{m,n} \phi_1^{m,n} + \Sigma_{r2}^{m,n} \phi_2^{m,n} + L_2^{n+1} = S_2^n
\]

As before it is assumed that the cross sections and flux terms can be written as follows:

Let: \( \Sigma_x^{m,n} = \Sigma_x^{m,n} + \delta \Sigma_x^m \) and \( \phi_g^{m,n} = \phi_g^{m,n} + \delta \phi_g^m \)
Placing these into equation (4-45):

\[ - (\Sigma_{12}^m(k) + \delta \Sigma_{12}^m) (\phi_1^m(k) + \delta \phi_1^m) + (\Sigma_{r2}^m(k) + \delta \Sigma_{r2}^m) (\phi_2^m(k) + \delta \phi_2^m) + L_2^n + 1 = S_2^n \]  

Multiplying through and getting rid of higher order terms the linearized form of the two group equation becomes:

\[ - \Sigma_{12}^m(k) \phi_1^m(k) - \Sigma_{12}^m \delta \phi_1^m + \Sigma_{r2}^m \phi_2^m(k) + \phi_2^m(k) \delta \Sigma_{r2}^m + \Sigma_{r2}^m \delta \phi_2 + L_2^n + 1 = S_2^n \]  

Expanding the cross sections in terms of the thermal hydraulic and feedback parameters and using the following compact notation:

\[ \frac{\partial \delta M_2}{\partial U} \delta U = \left[ \phi_2^m(k) \frac{\partial \Sigma_{r2}^m}{\partial \rho_m} - \phi_1^m(k) \frac{\partial \Sigma_{12}^m}{\partial \rho_m} \right] \left( \frac{\partial \rho_m}{\partial U} \right)^{(k)} \delta U \]

where: \( U = P, \alpha, T_g, T_p, P_a \)

\[ \frac{\partial \delta W_2}{\partial T_f} \delta T_f = \left[ \phi_2^m(k) \frac{\partial \Sigma_{r2}^m}{\partial T_f} - \phi_1^m(k) \frac{\partial \Sigma_{12}^m}{\partial T_f} \right] \delta T_f \]

The linearized form of the thermal group equation is given as:
Figure 4-1 shows a picture of the matrix for a 3x3x3 cartesian problem. This is not a real problem but a theoretical problem to demonstrate the matrix structure. This problem consists of 27 fluid cells each connected to a heat structure with two radial nodes. One heat conduction node represents the fuel rod clad and one node represents the fuel. Power is deposited in the fuel with 27 neutronics nodes. The coupling coefficients developed in this section are shown as the red, off-diagonal boxes. It can be seen from this picture the matrix is not symmetric and that it looks like something may be missing in the upper right hand corner of the picture. This is where the direct heating of the coolant terms would be, these terms are not considered at this time in the fully implicit coupling terms. Gamma heating is placed directly in the fluid based on the old time flux solution.
The convergence criteria used for the global flux for the new system of equations developed in this chapter is the same as in PARCS [24]. The first is based on the L2 norm of the difference of the new time and old time fission source term. The second uses the maximum fission source term residual. The two criteria are shown here for completeness.

\[
\delta_{L2} = \frac{\|\Psi^{m+1} - \Psi^m\|_2}{\langle \Psi^{n+1}, \Psi^n \rangle} \quad \text{and} \quad \delta_{L\infty} = \max \left| \frac{\Psi^{m,n+1} - \Psi^{m,n}}{\Psi^{m,n}} \right|
\]


4.3 Matrix Solution

In Chapter 2 the current temporal coupling between TRACE and PARCS was shown to be explicit in nature. The fluid equations are first solved, then the phasic temperatures and pressures are passed to the neutronics solver while the heat conduction equations use the liquid and vapor temperatures as boundary conditions to calculate the fuel temperature. The fuel temperature calculated by the heat conduction equation is then passed to the neutronics equation to calculate the neutron flux. In this coupling both the fluid equations and heat conduction equations are solved and converged on a solution before the neutronics equations are solved. The method presented here solves these systems and converge them all at the same time. The newly formed system of equations can become very large. The current direct solvers used in TRACE will not be capable of solving large systems of equations. In this section a strategy is developed to address the short comings of the current linear solver.

It is common practice to use a Newton method to linearize a set of equations and then solve the linearized set with a Krylov solver. In the literature review it was seen that a significant amount of research in this area utilized a Matrix Free or Jacobian Free Newton Krylov method. These methods were chosen in that research to avoid modifying the computer programs and the solvers currently implemented into the codes [38][24][8][11]. This research is not limited in this way and will not be limited to a matrix free method and is able to achieve full quadratic convergence.

As stated before the problem presented in this thesis involves the construction of one large matrix that will consist of the pressure matrix from TRACE, the temperature matrix from the heat conduction model in TRACE, the neutron flux matrix from PARCS, and all of the coupling terms shown in the previous section. The current solution method in TRACE uses a Newton iteration to converge the non-linear thermal-hydraulic/heat conduction system of equations. The pressure matrix is solved using the sparse direct matrix library SuperLU [39]. The SuperLU library is limited by the largest problem that can be solved on a single processor. For medium to large problems the SuperLU library is unable
to solve these problems. For example, the PBTT problem presented in Chapter 2 is a medium size problem but the fully formed matrix is very large. The neutronics model has 912 radial neutronics nodes in each of the 26 axial levels. They are mapped to 33 thermal-hydraulic channel components each consisting of 27 thermal hydraulics nodes, 9 radial heat conduction nodes, and 24 axial heat conduction nodes. The rest of the thermal-hydraulics model consists of a vessel (14 axial levels, 4 radial rings, 1 azimuthal sector) and 20 pipes, valves, tees, and pumps. This leads to a full matrix of almost 60,000 degrees of freedom. This large matrix will have to be solved using parallel solver. As part of this research several matrix solvers are used to determine speed and accuracy of different serial direct and iterative solvers. Three different linear solver packages are used, linpack full direct solver, SuperLU sparse direct solver and the linear solver package the Portable, Extensible Toolkit for Scientific Computation (PETSc). PETSc was chosen for its flexibility, speed, and stability. It is a mature software package and is used by approximately 230 computer codes ranging from nano-simulations and Biology/Medical to computational fluid dynamics and wave propagation simulations. This is a general purpose library for the solution of large, sparse, nonlinear systems of equations. This package contains a variety of Newton and Krylov subspace solvers. Figure 4-2 shows the calculational flow for a user based program that uses PETSc as a solver. The user supplies the routines for setting up the problem and calculating the jacobians. PETSc can handle time step, linear and nonlinear solution and preconditioning of the matrix [40][41][42].
PETSc is capable of running in serial and parallel. For parallel applications it uses standard Message Passing Interface (MPI) calls. Its design allows the user to generate parallel efficient solvers with minimal explicit writing of message passing code. It’s design is very flexible, it provides interfaces to a large number of external packages as well as allowing the user to generate customized solvers and data structures. A full listing of the external packages that PETSc already has an interface for can be found in Reference [40]. Figure 4-3 summarizes the numerical components distributed with PETSc. It is this flexibility that makes it possible for an in depth study to be done on different solvers and preconditioners.

Figure 4-2: Flow Control for the Solution of a PDE Using PETSc
To improve the convergence of Newton-Krylov methods, preconditioners are often employed as initial guesses at the solution. The closer to the actual solution the faster the convergence of the Newton-Krylov method will be. To successfully implement an efficient solver the preconditioners also needs to be investigated. PETSc also has an assortment of preconditioners that can be studied. However, the literature review has shown the best performance to come from physics based preconditioners. It is proposed here to use the current solutions in TRACE and PARCS as the preconditioners for the Newton-Krylov method. Figure 4-4 shows the program flow for this method.
The current solution of the coupled TRACE/PARCS the time-step is controlled by TRACE. The neutronics time-step advancement is then equal to the TRACE time-step. With the implicit coupling method the fast and thermal flux is also converged on during the outer Newton iteration. The new time-step size is based on the convergence of all independent parameters and takes into account the strong feedback parameters and limit time-step size when sharp gradients are present and larger time-step sizes when the transient is not as rapidly changing.

A small timing study was performed for each of the three solvers described above. The test problem used in this study consists of a Vessel (3 axial levels, 2 radial rings, 1 azimuthal sector), 2 pipes (5 cells), channel (27 thermal-hydraulic cells, 9 radial and 25 axial heat conduction nodes in the fuel rods), 25 neutronics nodes for active fuel height with two radial reflector nodes and one top and one bottom reflector node. The matrix size generated from this problem is 563 x 563. A steady state calculation is run and the CPU times are given in Table 4-1. The results in Table 4-1 show that PETSc is a very efficient for both direct and iterative solvers.
### Table 4-1: CPU times for different linear solvers

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<tr>
<th>Solver</th>
<th>CPU Time For Solver</th>
<th>Total CPU Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full Direct</td>
<td>30.9688</td>
<td>35.516</td>
</tr>
<tr>
<td>SuperLU</td>
<td>12.0000</td>
<td>16.312</td>
</tr>
<tr>
<td>PETSC (LU)</td>
<td>2.5156</td>
<td>6.828</td>
</tr>
<tr>
<td>PETSC (GMRES)</td>
<td>2.4375</td>
<td>6.984</td>
</tr>
</tbody>
</table>

#### 4.4 Summary

In this chapter the framework for an implicit method for solving the coupled system was established. This framework includes the cross section and power representation necessary for a consistent coupling of the equations from TRACE and PARCS. Also presented here is a general method resolving the nonlinearities introduced with the tightly coupled equations.
Chapter 5

RESULTS AND DISCUSSIONS

This chapter will present four simple test problems used to evaluate the implementation of implicit temporal coupling. Three of the test problems are representative of BWR problems and the fourth is representative of a PWR problem. These test problems will show the stability and improvements in accuracy that is achieved with the new implicit coupling. From this point forward the traditional coupling method will be referred to as the explicit method and the new method developed in the preceding chapters of this thesis will be referred to as the implicit method.

5.1 Test Problem Nodalization

The test problems used in this chapter use two different nodalizations, shown in Figure 5-1. Both of these models are simplified representations of fluid flow through a BWR or PWR rod bundle. A vertically oriented pipe component is connected to a fill at the bottom and a break at the top. The water in the pipe is heated with a heat structure which represents fuel rods. The fuel rods are powered by the neutronics nodes. The neutronics node in radial plane has the same dimensions as one fuel assembly for either a PWR or BWR.

The 3-cell nodalization is used to verify the coding for the implicit coupling and is used to test the numerical stability of the newly formed system. This nodalization consists of a pipe with 3 axial thermal hydraulic nodes connected to a fill at the bottom and a break at the top. Positive fluid flow is vertically upwards. The heat conduction has 4 radial cells and 3 axial cells. The three inner heat conduction cells are powered and the fourth is unpowered. The neutronics model has one node in the radial plane and three axial levels. The neutronics boundary conditions are reflective for both the radial and axial directions.
The 14-cell nodalization is used in the BWR turbine trip test problem and the PWR MSLB test problem. This nodalization is similar to the 3-cell except that the neutronics nodalization includes a top and bottom reflector with zero flux boundary conditions. The axial node dimensions used in the 14-cell problem are more realistic, the axial node height is similar to the radial dimension of a fuel rod bundle for either a PWR or BWR.

5.2 Simple Test Problems Representative of BWR

The first set of test problems utilize the 3-cell nodalization shown in Figure 5-1. For all of these test problems a stand alone TRACE calculation is run to obtain steady state
conditions for the thermal hydraulics model assuming a constant power. A coupled
TRACE/PARCS calculation is run, restarting from the standalone results to obtain cou-
pled steady state results. The coupled steady state results are then used as a starting point
for the transient simulations. Steady state for the BWR test problems are obtained using a
fill temperature of 548 K and a liquid velocity of 0.98 m/s. The break pressure is 6.83E6
Pa.

5.2.1 Numerical Stability

Null Transient

The first test problem presented here is the calculation of a null transient. A null tran-
sient is a time dependent solution without perturbing the system. The results of a null
transient should result in the reproduction of the steady state results. However, in a null
transient the power is no longer a boundary condition and is allowed to change with
changing thermal hydraulic conditions. Therefore, small variations in thermal-hydraulic
parameters, fuel temperatures, or power can lead to numeric instabilities at large time step
sizes. This is especially true for the explicit temporal coupling between TRACE and
PARCS.

The null transient is run with the maximum time step size set to 1.0. TRACE will
automatically adjust the time step size based on the convergence of the thermal hydraulic
parameters, for the explicit coupling. Figure 5-2 shows the development of a numerical
instability in the explicit coupling. The black line in this figure shows that the instability
grow from the steady state value and become completely unstable after about 5 seconds.
Once the numerical instability happens it remains unstable and oscillates between a maxi-
mum and minimum value. Figure 5-3 shows how TRACE attempts to reduce the time
step size as the numerical instability develops. The same numerical experiment was con-
ducted using the implicit temporal coupling. The results of this calculation are shown in
Figure 5-2 as the red line. The red line shows that the implicit coupling results in a stable
solution. Figure 5-3 also shows that the implicit temporal coupling is able to maintain the largest time step size for this problem.

Figure 5-2: Explicit Coupling Numeric Instabilities in Null Transient

Figure 5-3: Time Step Size for Numeric Instabilities in Null Transient
Temperature Transient

A similar numerical experiment is conducted by varying the fill temperature as shown in Figure 5-4. This transient is run by starting from the same initial conditions as the previous numerical experiment. The fill temperature is linearly decreased from 548 K to 530 K in over one second it is held constant for 6 seconds then increased back to the original 548 K in a tenth of a second.

The colder water entering the core causes the void distribution to decrease, the density of the water to increase and results in over moderation of the core. The power subsequently increases until the temperature of the water entering the core is restored. The power then returns to the original steady state value. The transients are once again run setting the maximum time step size to 1.0. The results for both the explicit and implicit temporal coupling methods is shown in Figure 5-5. As expected the explicit coupling solution goes unstable and remains unstable throughout the entire transient. The implicit coupling remains stable throughout the entire transient.
Figure 5-5: Instabilities in Power for Temperature Transient

Figure 5-6: Time Step Size for Temperature Transient

Figure 5-6 shows the time step size variation for this transient. During the rapid power change the implicit coupling reduces the time step size. This results in a stable and accurate power prediction. The time step size then automatically increases as the rate of
change in power decreases. To obtain a stable solution for the explicit coupling case the maximum time step size has to be reduced to 0.075 seconds.

5.2.2 Simple Test Problems Representative of BWR Turbine Trip Accident

This set of test problems use both the 3-cell and 14-cell nodalizations to simulate a power response similar to a BWR turbine trip accident. The transient is initiated by changing the break pressure as shown in Figure 5-7. This pressure boundary condition is applied to both the 3-cell and 14-cell problems. The rapid pressure increase is meant to simulate the steam line valve closing and then decreasing with the opening of relief valves. During this transient the large pressure spike causes the voids to collapse in the core resulting in a rapid power excursion. As shown in Chapter 2 the peak power is hard to predict. The magnitude of the peak varies widely with time step size. For both of these transients the maximum time step size is varied to determine the height of the peak power.

Figure 5-7: Break Pressure for Transient
3-Cell Numerical Experiment

Figure 5-8 and Figure 5-9 show the power and void variation with time step size for the explicit coupling. At large time step sizes large variations are seen as before. As the time step size is reduced the peak power converges to the power shape shown by the blue dotted line. Figure 5-10 and Figure 5-11 show the implicit results for this transient. For comparison the results are plotted on the same scale as those for the explicit case. Also shown on this plot is the smallest time step results for the explicit coupling. Both implicit and explicit models converge on this solution as time step size is decreased. The variation in the peak power prediction is significantly reduced for the implicit temporal coupling. The percentage shown in the power figures compare the peak power at each time step size to the peak power at the explicit curve at time step size 0.001. It can also be seen that the implicit calculations converge on the final solution at a larger time step.
Figure 5-9: Explicit Coupling Void Variation for Pressure Transient

Figure 5-10: Implicit Coupling Power Variation for Pressure Transient - 3-Cell
14-Cell Numerical Experiment

The same set of transients are run with the 14-cell model. Figure 5-12 and Figure 5-13 show the results for the explicit and implicit calculations respectively. The explicit results show a significant reduction in the peak power variation. The implicit results show very little variation in the peak power prediction. Both of these sets of calculations show that accurate results can be obtained with larger maximum time step size.
Figure 5-12: Explicit Coupling Power Variation for Pressure Transient - 14-cell

Figure 5-13: Implicit Coupling Power Variation for Pressure Transient - 14-Cell
5.3 Simple Test Problem Representative of PWR

The final test problem utilize 14-cell nodalization shown in Figure 5-1. This test problem is representative of a PWR. As before a stand alone TRACE calculation is run to obtain steady state conditions for the thermal hydraulics model assuming a constant power. A coupled TRACE/PARCS calculation is run, restarting from the standalone results to obtain coupled steady state results. The coupled steady state results are then used as a starting point for the transient simulations. Steady state for the PWR test problems are obtained using a fill temperature of 562 K and a liquid velocity of 4.95 m/s. The break pressure is 1.58E7 Pa.

5.3.1 Simple Test Problem Representative of PWR Main Steam Line Accident

The main steam line accident is characterized by a slug of cold water entering the reactor causing the power to increase. The reactor scrams on 114% power. After the scram the water entering the reactor continues to decrease. The over cooling causes a return to power. This same behavior is achieved in this test problem by varying the fill temperature as shown in Figure 5-14.
Figure 5-14: Fill Temperature for PWR Transient

Figure 5-15: Reactor Power for PWR Transient
Figure 5-15 and Figure 5-16 show the power and time step size for the explicit and implicit coupling. In Chapter 2 it was shown that for the full scale TMI MSLB accident variations in the peak power location and subsequent return to power are dependent on time step size. Those results could not be replicated using this simple problem. Figure 5-15 shows that both coupling methods have the same results. Figure 5-16 shows that both explicit and implicit run at approximately the same time step size. There is some variation in time step size during the return to power portion of the transient. However, this variation is very small and is in the fifth decimal place of the time step size. Even though this test problem did not show any dependence on time step size for one channel it does show that this method can accurately calculate the results for a more detailed calculation with a reactor scram.
5.4 Summary

The results presented in this chapter show that the implicit coupling method for the test problems shown is numerically stable. They also show that the coupling is capable of accurately simulating the power response for transients for both PWR and BWR simulations. They show that on average a large time step can be taken to achieve a comparable level of accuracy with the explicit method.
Chapter 6

CONCLUSIONS AND FUTURE WORK

The purpose of this research was to improve the stability and accuracy of coupled multi-physics calculations by removing the error associated with the explicit treatment of the feedback terms passed between the different physics codes. A numerical study was preformed using the coupled reactor analysis code TRAC/E/PARCS. The study utilized well documented OECD benchmark problems; Peach Bottom TT and OECD/NRC TMI MSLB. These accidents were analyzed to determine their sensitivity to time step size. This study showed that the explicit treatment of the feedback terms caused large variations in the peak power predicted in transients with rapid power excursions (PB TT), Figure 2-13 and Figure 2-14, as well as the location and magnitude of power in longer running calculations (TMI MSLB), Figure 2-8 through Figure 2-11. The study also showed that small time steps were required to obtain accurate result. The time step size and duration have to be determined by the user.

Previous attempts at removing these errors showed limited success. Jacobian free and nested loop methods were attempted in the past since these methods are easier to implement. They do not require large modifications of the individual code package. Because of the simplifications with these methods, convergence of all parameters is not guaranteed. It was determined that the most appropriate strategy to solving this problem correctly was to form a full set of consistent tightly coupled equations. By approaching the problem in this manner we reduce errors associated with the uncertainly of the coupled method and maintain quadratic convergence.

The first step to forming the full system matrix is to obtain the coefficient matrix for the thermal hydraulics, heat conduction, and neutronics equations. Once these coefficients were collected the non-linear terms could be added to the equation set. These equa-
tion sets are then written in terms of a consistent set of unknowns and linearized using a first order approximation. This requires that derivatives of the cross sections with respect to fuel temperature and moderator density be calculated. This is required since the cross section libraries used in this analysis are based on fuel temperature and moderator density only. However, the thermal hydraulic variables used in the equation set are total pressure, void fraction, vapor temperature, liquid temperature, and non-condensable gas pressure. This requires and additional linearization of the density in terms of these parameters. This is also true for the power deposited in the heat structure, which is dependent on both the flux and the fission cross section. This results in a significant number of off diagonal terms for both the neutronics equations and the heat conduction equations, shown in Figure 6-1. The computational flow is controlled by TRACE in the explicit method, and has a Newton iteration built in already. The convergence of the flux is added to the outer iteration convergence, thus completing the integration of the neutronics equation set.

The simple test problems presented in Chapter 5 demonstrate the accuracy and stability of the method developed in this research. The study showed that the time step size changed with the fastest moving physics. This means that the accuracy of the results can be achieved at the largest time step based on the convergence of all the physics phenomena. Two representative test problems were developed and analyzed based on the Peach Bottom turbine trip accident and Three Mile Island main steam line break accident. These test problems verified the ability of the new coupled code to accurately predict the power response during fast and long running transients. The Peach Bottom test problem also showed significant reduction in the dependence of the peak power prediction on time step size.

The use of small problems shows that significant improvements can be achieved when the implicit coupling is used for larger full scale analysis problems. However, technical challenges remain that have prevented this from being fully realized. The technical challenges are primarily caused by the large size of the fully formed coupled matrix. For example, Figure 6-1 shows the full matrix for the Peach Bottom Turbine Trip accident.
The matrix size is approximately 60,000 x 60,000 with almost a million non-zero elements.

This matrix is dominated by the neutronics solution. There are more than 40,000 equations associated with the neutronics solution. The complexity of the off diagonal coupling terms can also be readily seen. This creates a very complex sparse matrix structure. It is not possible to solve this matrix with the tools presented in this research. Only serial versions of the solvers were used on a 32 bit architecture. To solve matrices this large efficiently parallel solvers will have to be used. Another technical challenge with matrices
this large is that they need to be stored in a compressed format. The method implemented in this research does not load the array into a data structure that is easily converted to a sparse data format. Therefore a sort of the matrix is required before the data is passed to the solver. This sort becomes very expensive for large matrices. This problem can be overcome by predetermining all potential non-zero matrix locations and filling the data structure with the appropriate sparse data structure. This will eliminate the need for a sort before the solver.

A study should be conducted to determine the most appropriate solver for a system of equations this large and larger. In the example shown in Figure 6-1 a full nodalization of the reactor core is coupled to 33 channel components. There is a desire to increase the number of channels to match the number of neutronics nodes. This means both the thermal hydraulics and heat conduction portion of the matrix will become as large or larger than the neutronics portion shown above. This will result in matrices with well over 100,000 degrees of freedom. To solve matrices this large parallel iterative Krylov solvers will be required.
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<thead>
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<th>Reference</th>
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<tr>
<td>41</td>
<td>S. Baley, et. al., “PETSc Users Manual”, Argonne National Laboratory, ANL-95/11 - Revision 2.3.3, 2007</td>
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Appendix A

FINITE DIFFERENCE FORMULATIONS FOR THE FLUID AND TEMPERATURE EQUATIONS

This appendix lists the finite difference formulations for the equations discussed in this dissertation.

A.7 3-D Finite-Difference equations

This derivation uses an orthogonal, right-handed, cylindrical coordinate system.

A.7.1 Gas Momentum:

Axial Component:

\[
\alpha \rho_g \left( \frac{\partial V_{gz}}{\partial t} + V_{gr} \frac{\partial V_{gz}}{\partial r} + \frac{V_{g\theta}}{r} \frac{\partial V_{gz}}{\partial \theta} + V_{gz} \frac{\partial V_{gz}}{\partial z} \right) = -\alpha \frac{\partial P}{\partial z} - \alpha \rho_g g_z - f_{iz} + f_{wgz} \tag{A-1}
\]

\[
\frac{\partial V_{gz}}{\partial t} + V_{gr} \frac{\partial V_{gz}}{\partial r} + \frac{V_{g\theta}}{r} \frac{\partial V_{gz}}{\partial \theta} + V_{gz} \frac{\partial V_{gz}}{\partial z} = -\frac{1}{\rho_g} \frac{\partial P}{\partial z} - g_z + \frac{(-f_{iz} + f_{wgz})}{\alpha \rho_g} \tag{A-2}
\]

\[
\left[ V_{g}^{n+1} - V_{g}^{n+1} \right] \bigg|_{r, \theta, z + 1/2} + \left[ V_{g \cdot V_{g}^{n+1}} \right] \bigg|_{r, \theta, z + 1/2} = \frac{1}{\Delta t} \left[ P_{n+1}^{(r, \theta, z + 1)} - P_{n+1}^{(r, \theta, z)} \right] - g_z \Delta h(z) + \frac{(-f_{iz} + f_{wgz})}{\langle \alpha \rho_g \rangle} \tag{A-3}
\]
\[
\left[ \frac{V_{g}^{n+1} - V_{g}^{n}}{\Delta t} \right]_{r, 0, z+1/2} + \left[ V_{gr} \frac{\Delta r V_{gr}^{n+1}}{\Delta r} + \frac{V_{g0} \Delta \theta V_{gr}^{n+1}}{r} + V_{gz} \frac{\Delta z V_{gr}^{n+1}}{\Delta z} \right]_{r, 0, z+1/2} \\
= - \frac{1}{\langle \rho^{n}_{g} \rangle} \frac{P^{n+1}(r, \theta, z+1) - P^{n+1}(r, \theta, z)}{\Delta z} - g_{z} \Delta h(z) + \frac{(-f_{iz} + f_{wgr})}{\langle \alpha^{n} \rho^{n}_{g} \rangle}
\] (A-4)

Radial Component:

\[
\alpha \rho_{g} \left( \frac{\partial V_{gr}}{\partial t} + \frac{\partial V_{gr}}{\partial r} + \frac{V_{g0} \partial V_{gr}}{r \partial \theta} - \frac{V_{gr}^{2}}{r} + V_{gz} \frac{\partial V_{gr}}{\partial z} \right) \\
= - \alpha \frac{\partial P}{\partial r} - \alpha \rho_{g} g_{r} - f_{ir} + f_{wgr}
\] (A-5)

\[
\frac{\partial V_{gr}}{\partial t} + \frac{\partial V_{gr}}{\partial r} + \frac{V_{g0} \partial V_{gr}}{r \partial \theta} - \frac{V_{gr}^{2}}{r} + V_{gz} \frac{\partial V_{gr}}{\partial z} = - \frac{1}{\rho_{g} \partial r} - g_{r} + \frac{(-f_{ir} + f_{wgr})}{\alpha \rho_{g}}
\] (A-6)

\[
\left[ \frac{V_{g}^{n+1} - V_{g}^{n}}{\Delta t} \right]_{r+1/2, 0, z} + \left[ V_{gr} \nabla \cdot V_{gr}^{n+1} \right]_{r+1/2, 0, z} = \\
- \frac{1}{\langle \rho^{n}_{g} \rangle} \frac{P^{n+1}(r+1, \theta, z) - P^{n+1}(r, \theta, z)}{\Delta r} - g_{r} \Delta h(r) + \frac{(-f_{ir} + f_{wgr})}{\langle \alpha^{n} \rho^{n}_{g} \rangle}
\] (A-7)

\[
\left[ \frac{V_{g}^{n+1} - V_{g}^{n}}{\Delta t} \right]_{r+1/2, 0, z} + \left[ V_{gr} \frac{\Delta r V_{gr}^{n+1}}{\Delta r} + \frac{V_{g0} \Delta \theta V_{gr}^{n+1}}{r} + V_{gz} \frac{\Delta z V_{gr}^{n+1}}{\Delta z} \right]_{r+1/2, 0, z} \\
= - \frac{1}{\langle \rho^{n}_{g} \rangle} \frac{P^{n+1}(r+1, \theta, z) - P^{n+1}(r, \theta, z)}{\Delta r} - g_{r} \Delta h(r) + \frac{(-f_{ir} + f_{wgr})}{\langle \alpha^{n} \rho^{n}_{g} \rangle}
\] (A-8)
Azimuthal Component:

\[
\alpha \rho_g \left( \frac{\partial V_{g\theta}}{\partial t} + V_{gr} \frac{\partial V_{g\theta}}{\partial r} + \frac{V_{g\theta} V_{gr} V_{r\theta}}{r} + V_{gz} \frac{\partial V_{g\theta}}{\partial z} \right) = -\frac{\alpha \partial P}{r \partial \theta} - \alpha \rho_g g_0 f_{i\theta} + f_{w_{g\theta}} \tag{A-9}
\]

\[
\frac{\partial V_{g\theta}}{\partial t} + V_{gr} \frac{\partial V_{g\theta}}{\partial r} + \frac{V_{g\theta} V_{gr} V_{r\theta}}{r} + V_{gz} \frac{\partial V_{g\theta}}{\partial z} = -\frac{1}{r \rho_g \partial \theta} - g_0 + \frac{(-f_{i\theta} + f_{w_{g\theta}})}{\alpha \rho_g} \tag{A-10}
\]

\[
\left[ \frac{V_{g}^{n+1} - V_{g}^{n}}{\Delta t} \right]_{r, \theta+1/2, z} + \left[ V_{gr} \nabla \cdot V_{g}^{n+1} \right]_{r, \theta+1/2, z} = \left[ V_{g}^{n+1} - V_{g}^{n} \right]_{r, \theta+1/2, z} \tag{A-11}
\]

\[
-\frac{1}{\left\langle \rho^n_g \right\rangle} P^n_{r, \theta+1, z} - P^n_{r, \theta, z} - g_0 \Delta h(\theta) + \frac{(-f_{i\theta} + f_{w_{g\theta}})}{\left\langle \alpha^n \rho^n_g \right\rangle} \tag{A-12}
\]

\[
\left[ V_{g}^{n+1} - V_{g}^{n} \right]_{r, \theta+1/2, z} \Delta t
\]

\[
\left[ V_{gr} \frac{\Delta V_{g\theta}^{n+1}}{\Delta r} + \frac{V_{g\theta} \Delta V_{g\theta}^{n+1}}{\Delta \theta} + \frac{V_{gz} \Delta V_{g\theta}^{n+1}}{\Delta z} \right]_{r, \theta+1/2, z} = \left[ V_{gr} \frac{\Delta V_{g\theta}^{n+1}}{\Delta r} + \frac{V_{g\theta} \Delta V_{g\theta}^{n+1}}{\Delta \theta} + \frac{V_{gz} \Delta V_{g\theta}^{n+1}}{\Delta z} \right]_{r, \theta+1/2, z}
\]

\[
-\frac{1}{\left\langle \rho^n_g \right\rangle} P^n_{r, \theta+1, z} - P^n_{r, \theta, z} - g_0 \Delta h(\theta) + \frac{(-f_{i\theta} + f_{w_{g\theta}})}{\left\langle \alpha^n \rho^n_g \right\rangle} \tag{A-12}
\]

1.1.1 Liquid Momentum:

Axial Component:

\[
(1 - \alpha) \rho \left( \frac{\partial V_{lz}}{\partial t} + V_{lr} \frac{\partial V_{lz}}{\partial r} + \frac{V_{l\theta} \partial V_{lz}}{\partial \theta} + V_{lz} \frac{\partial V_{lz}}{\partial z} \right) = -(1 - \alpha) \frac{\partial P}{\partial z} - (1 - \alpha) \rho g_0 + f_{iz} - f_{w_{iz}} \tag{A-13}
\]
\[
\frac{[V_t^{n+1} - V_t^n]}{\Delta t}_{r, \theta, z + 1/2} + [V_{lr} \nabla \cdot V_{lr}^{n+1}]_{r, \theta, z + 1/2} = \]
(A-14)
\[
- \frac{1}{\langle \rho_t^n \rangle} \frac{P^{n+1}(r, \theta, z + 1) - P^{n+1}(r, \theta, z)}{\Delta z} - g_2 \Delta h(z) + \frac{(-f_{iz} + f_{wlz})}{\langle (1 - \alpha^n) \rho_t^n \rangle}
\]
\[
\frac{[V_t^{n+1} - V_t^n]}{\Delta t}_{r, \theta, z + 1/2} = \]
(A-15)
\[
+ \left[ V_{lr} \frac{\Delta r V_{lr}^{n+1}}{\Delta r} + V_{l0} \frac{\Delta \theta V_{lr}^{n+1}}{\Delta \theta} + V_{lz} \frac{\Delta z V_{lz}^{n+1}}{\Delta z} \right]_{r, \theta, z + 1/2}
\]
\[
- \frac{1}{\langle \rho_t^n \rangle} \frac{P^{n+1}(r, \theta, z + 1) - P^{n+1}(r, \theta, z)}{\Delta z} - g_2 \Delta h(z) + \frac{(-f_{iz} + f_{wlz})}{\langle (1 - \alpha^n) \rho_t^n \rangle}
\]

Radial Component:

\[
(1 - \alpha) \rho_t \left( \frac{\partial V_{lr}}{\partial t} + \nabla_{lr} \cdot \nabla_{lr} \rho_t - \frac{V_{l0}}{r} \frac{\partial V_{lr}}{\partial r} - V_{l0} \frac{\partial V_{lr}}{\partial \theta} - \frac{V_{lz}^2}{r} + V_{lz} \frac{\partial V_{lr}}{\partial z} \right) =
\]
(A-16)
\[
- (1 - \alpha) \frac{\partial P}{\partial r} - (1 - \alpha) \rho_t g_r - f_{ir} + f_{wlr}
\]
\[
\frac{[V_t^{n+1} - V_t^n]}{\Delta t}_{r + 1/2, \theta, z} + [V_{lr} \nabla \cdot V_{lr}^{n+1}]_{r + 1/2, \theta, z} = \]
(A-17)
\[
- \frac{1}{\langle \rho_t^n \rangle} \frac{P^{n+1}(r + 1, \theta, z) - P^{n+1}(r, \theta, z)}{\Delta r} - g_r \Delta h(r) + \frac{(-f_{ir} + f_{wlr})}{\langle (1 - \alpha^n) \rho_t^n \rangle}
\]
\[ \frac{[V_{l}^{n+1} - V_{l}^{n}]}{\Delta t}_{r+1/2, 0, z} \]

\[ + \left[ V_{lr} \frac{\Delta r V_{lr}^{n+1}}{\Delta r} + \frac{V_{i0} \Delta z V_{lr}^{n+1}}{\Delta \theta} - \frac{V_{i0}^2}{r} + V_{lz} \frac{\Delta z V_{lr}^{n+1}}{\Delta z} \right] \]

\[ = \]

\[ \frac{1}{\langle \rho_l^n \rangle} \frac{P^n(r + 1, \theta, z) - P^n(r, \theta, z)}{\Delta t} - g \Delta h(r) + \frac{(-f_{ir} + f_{wlr})}{\langle (1 - \alpha^n) \rho_l^n \rangle} \]

Azimuthal Component:

\[ (1 - \alpha) \rho_l \left( \frac{\partial V_{i0}}{\partial t} + \frac{V_{i0} \partial V_{i0}}{r} + \frac{V_{lr} \partial V_{i0}}{\partial \theta} + \frac{V_{i0} V_{lr}}{r} + \frac{V_{i0} V_{i0}}{r} \right) = \]

\[ - \frac{(1 - \alpha) \partial P}{r} - (1 - \alpha) \rho_0 g - f_{ir} + f_{wlr} \]

\[ \frac{[V_{l}^{n+1} - V_{l}^{n}]}{\Delta t}_{r, 0 + 1/2, z} + \left[ V_{lr} \nabla \cdot \frac{V_{i0}^{n+1}}{\Delta \theta} \right]_{r, 0 + 1/2, z} = \frac{1}{\langle \rho_l^n \rangle} \frac{P^n(r + 1, \theta, z) - P^n(r, \theta, z)}{\Delta \theta} - g \Delta h(\theta) + \frac{(-f_{i0} + f_{wg0})}{\langle (1 - \alpha^n) \rho_l^n \rangle} \]

\[ \frac{[V_{l}^{n+1} - V_{l}^{n}]}{\Delta t}_{r, 0 + 1/2, z} = \]

\[ + \left[ V_{lr} \frac{\Delta r V_{lr}^{n+1}}{\Delta r} + \frac{V_{i0} \Delta z V_{lr}^{n+1}}{\Delta \theta} - \frac{V_{i0}^2}{r} + V_{lz} \frac{\Delta z V_{lr}^{n+1}}{\Delta z} \right] \]

\[ - \frac{1}{\langle \rho_l^n \rangle} \frac{P^n(r + 1, \theta, z) - P^n(r, \theta, z)}{\Delta \theta} - g \Delta h(\theta) + \frac{(-f_{i0} + f_{wg0})}{\langle (1 - \alpha^n) \rho_l^n \rangle} \]
1.1.2 Gas Mass

\[ \frac{\partial \alpha \rho g}{\partial t} + \nabla \cdot (\alpha \rho g \hat{v}_g) = \Gamma_i \quad (A-22) \]

\[ \left[ \alpha^n \rho g^n - \alpha^n \rho g^n \right]_{r, \theta, z} \left[ \nabla \cdot (\alpha^n \rho g^n \hat{v}_g^n) \right]_{r, \theta, z} = \Gamma^n + 1 \quad (A-23) \]

1.1.3 Liquid Mass

\[ \frac{\partial (1 - \alpha) \rho l}{\partial t} + \nabla \cdot [(1 - \alpha) \rho l \hat{v}_l] = -\Gamma_i \quad (A-24) \]

\[ \left[ (1 - \alpha) \rho l^n - (1 - \alpha) \rho l^n \right]_{r, \theta, z} \left[ \nabla \cdot ((1 - \alpha) \rho l^n \hat{v}_l^n) \right]_{r, \theta, z} = -\Gamma^{n+1} \quad (A-25) \]

1.1.4 Non condensable Gas:

\[ \frac{\partial \alpha \rho a}{\partial t} + \nabla \cdot (\alpha \rho a \hat{v}_a) = \Gamma_i \quad (A-26) \]

\[ \left[ \alpha^n \rho a^n - \alpha^n \rho a^n \right]_{r, \theta, z} \left[ \nabla \cdot (\alpha^n \rho a^n \hat{v}_a^n) \right]_{r, \theta, z} = 0 \quad (A-27) \]
1.1.5 Gas Energy:

\[
\frac{\partial}{\partial t} (\alpha \rho_g e_g) + \nabla \cdot (\alpha \rho_g e_g \hat{\nu}_g) = -P \left[ \frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \hat{\nu}_i) \right] + \Gamma h_{fg} + q_{wg} + q_{ig} + q_{dg}
\]  

(A-28)

\[
\frac{[\alpha^{n+1} \rho_{g}^{n+1} e_{g}^{n+1} - \alpha^{n} \rho_{g}^{n} e_{g}^{n}]}{\Delta t} \bigg|_{r, \theta, z} + \left[ \nabla \cdot (\alpha^{n} \rho_{g}^{n} e_{g}^{n} \hat{\nu}_{g}^{n+1}) \right] \bigg|_{r, \theta, z} = \frac{\alpha^{n+1} - \alpha^{n}}{\Delta t} \bigg|_{r, \theta, z}
\]  

(A-29)

\[
- P^{n+1} \left[ \frac{[\alpha^{n+1} - \alpha^{n}]}{\Delta t} + \nabla \cdot (\alpha^{n} \hat{\nu}_{g}^{n+1}) \right] \bigg|_{r, \theta, z} + \Gamma^{n+1} h_{fg}^{n+1} + q_{wg}^{n+1} + q_{ig}^{n+1} + q_{dg}^{n+1}
\]

1.1.6 Mixture Energy:

\[
\frac{\partial}{\partial t} [\alpha \rho_{g} e_{g} + (1 - \alpha) \rho_{l} e_{l}] + \nabla \cdot [\alpha \rho_{g} e_{g} \hat{\nu}_{g} + (1 - \alpha) \rho_{l} e_{l} \hat{\nu}_{l}] = -P \nabla \cdot [\alpha \hat{\nu}_{g} + (1 - \alpha) \hat{\nu}_{l}] + q_{wg} + q_{wl} + q_{dg} + q_{dl}
\]  

(A-30)

\[
\frac{[\alpha^{n+1} \rho_{g}^{n+1} e_{g}^{n+1} + (1 - \alpha^{n+1}) \rho_{l}^{n+1} e_{l}^{n+1} - \alpha^{n} \rho_{g}^{n} e_{g}^{n} - (1 - \alpha^{n}) \rho_{l}^{n} e_{l}^{n}]}{\Delta t} \bigg|_{r, \theta, z} + \left[ \nabla \cdot (\alpha^{n} \rho_{g}^{n} e_{g}^{n} \hat{\nu}_{g}^{n+1}) \right] \bigg|_{r, \theta, z} + P^{n+1} \nabla \cdot [\alpha^{n} \hat{\nu}_{g}^{n+1} + (1 - \alpha^{n}) \hat{\nu}_{l}^{n+1}] \bigg|_{r, \theta, z} = q_{wg}^{n+1} + q_{wl}^{n+1} + q_{ig}^{n+1} + q_{dg}^{n+1}
\]  

(A-31)
Where:

\[ q_{wg}^{n+1} = h_{wg}^n a_w (T_{wg}^{n+1} - T_g^{n+1}) \]  \hspace{1cm} (A-32)

\[ q_{wl}^{n+1} = h_{wl}^n a_w (T_{wl}^{n+1} - T_l^{n+1}) \]  \hspace{1cm} (A-33)

1.1.7 Heat Conduction:

\[ \rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q'' \]  \hspace{1cm} (A-34)

\[ \left\{ \left( \rho C_p \right)_{ij} \frac{T_{ij}^{n+1} - T_{ij}^n}{\Delta t} - q''_{ij} \right\} \frac{1}{2} \left[ \left( r_i \Delta r_i + \frac{\Delta r_i^2}{4} \right) + \left( r_{i-1} \Delta r_{i-1} - \frac{\Delta r_{i-1}^2}{4} \right) \right] \frac{\Delta z_j + \Delta z_{j-1}}{2} \]  \hspace{1cm} (A-35)

\[ = \left\{ r_{i+1/2} k_{i+1/2, j} \left( \frac{T_{i+1,j}^{n+1} - T_{ij}^{n}}{\Delta r_i} \right) + r_{i-1/2} k_{i-1/2, j} \left( \frac{T_{i-1,j}^{n+1} - T_{ij}^{n}}{\Delta r_{i-1}} \right) \right\} \]

\[ \times \frac{\Delta z_j + \Delta z_{j-1}}{2} + \left\{ k_{i,j+1/2} \left( \frac{T_{i,j+1}^{n} - T_{ij}^{n}}{\Delta z_j} \right) + k_{i,j-1/2} \left( \frac{T_{i,j-1}^{n} - T_{ij}^{n}}{\Delta z_{j-1}} \right) \right\} \]

\[ \times \frac{1}{2} \left[ \left( r_i \Delta r_i + \frac{\Delta r_i^2}{4} \right) + \left( r_{i-1} \Delta r_{i-1} - \frac{\Delta r_{i-1}^2}{4} \right) \right] \]
Appendix B

SAMPLE TRACE AND PARCS INPUT FILES FOR THE TEST PROBLEMS

This appendix lists the TRACE and PARCS input files for each of the base test problems used in this dissertation.

B.2 3-Node Test Problem Representative of a BWR

TRACE Steady State Input File

free format
*
*
*************
* main data *
*************
*
  numtcr     ieos     inopt    nmat    id2o
  2           0         1        0        0
This is a test problem for my thesis. It represents a small BWR channel.
*
*
*************
* namelist data *
*************
*
&inopts
cpuflg=1,
ittmr=0,
n solver=1,
usesjc=3,
npower=1,
nhtstr=1,
nosets=1,
nCouple=0
&end
*
*************
* Model Flags *


***************
*  
*       dstep      timet
*          0     0.0
*  stdyst     transi      ncomp      njun      ipak
*           1       0       5       2       1
*  epso      epss
*      1.0E-3    1.0E-10
*  oitmax     sitmax      isolut      ncontr      nccf1
*           10      10       0       0       0
*  ntsv      ntcb      ntcf      ntrp      ntcp
*           1       0       0       1       0
*  
****************************************************
*   component-number data  *
****************************************************
*  Component input order (IORDER)  *
*---- type ---- num ------------- name ----------------  +    jun1  
*jun2  jun3  
*      FILL      *      1 s      *      velocity bc      +       1
*      PIPE      *      2 s      *      subcooled liquid channel      +       1       3
*      BREAK      *      3 s      *      pressure bc      +       3
*      HTSTR      *      4 s      *      powered-rod conductor      +
*      POWER      *    901 e      *      power data input test1      +
*  
****************************************************
*   Starting Signal Variable Section of Model  *
****************************************************
*  
*         idsv      isvn      ilcn      icn1      icn2
*           1       0       0       0       0
****************************************************
*   Finished Signal Variable Section of Model  *
****************************************************
*  
*  **************************************
*   Starting Trip Section of Model  *
*  **************************************
*  
* Trip Storage Count Card  *
*   ntse      ntct      ntsf      ntdp      ntsd
*           0       0       0       0       0
*  
*trip
*  
*   idtp      isrt      iset      itst      idsg
*  -2       2       0       1       1
*setp(1)      setp(2)
*  0.0       0.1
*   dtsp(1)      dtsp(2)
********** type  num  userid  component name
  fill 1     1                    velocity bc
  *      jun1  ifty  ioff
        1     2     0
  *      twtold  rfmx  concin  felv
         0.0    0.0    0.0         0.0
  *      dxin  volin  alpin  vlin  tlin
         1.0  0.0491    0.0         0.0         548.0
  *      pin  pain  flowin  vvin  tvin
       6.88405E6    0.0     7.5         0.0         548.0

********** type  num  userid  component name
  pipe 2     1       subcooled liquid channel
  *      ncells  nodes  jun1  jun2  epsw
           5     0     1     3         0.0
  *      nsides
         0
  *      ichf  iconc  pipetype  ipow  npipes
           1     0     0     0         1
  *      radin  th  houtl  houtv  toutl
         0.0    0.0    0.0         0.0         0.0
  *      toutv  pwin  pwoff  rpwmx  pwsc1
        0.0    0.0    0.0         0.0         0.0
  dx  *     1.0     1.4     1.4     1.4s
  *      dx  *     1.0e
  vol  *    0.0491  0.0687  0.0687  0.0687s
  *      vol  *    0.0491e
  fa  *     0.01    0.01    0.01     0.01s
  *      fa  *     0.01    0.01e
  fric  *    0.0    0.0    0.0     0.0s
  *      fric  *    0.0    0.0e
  grav  *    1.0    1.0    1.0     1.0s
  *      grav  *    1.0    1.0e
  hd  *    1.0    1.4    1.4     1.4s
  *      hd  *    1.4    1.0e
  nff  *     0     0     0          0s
  *      nff  *     0     0e
  alp  *    0.0    0.01    0.01     0.01s
* alp * 0.18e
* vl * 0.0 0.0 0.0 0.0s
* vl * 0.0 0.0e
* vv * 0.0 0.0 0.0 0.0s
* vv * 0.0 0.0e
* tl * 548.0 558.0 558.0 558.0s
* tl * 558.0e
* tv * 558.0 558.0 558.0 558.0s
* tv * 558.0e
* p * 6.92E6 6.92E6 6.92E6 6.92E6s
* p * 6.92E6e
* pa * 0.0 0.0 0.0 0.0s
* pa * 0.0e

****** type num userid component name
break 3 1 pressure bc
* jn1 ibty isat ioff adjpress
  3 0 0 0 0
* dxin volin alpin tin pin
  1.0 0.0491 1.0 558.0 6.82972E6
* pain concin rbmx poff belv
  0.0 0.0 0.0 0.0 0.0

********** Starting Heat Structure Section of Model **********

****** type num userid component name
htstr 4 0 powered-rod conductor
* nhstr ittc hscyl ichf
  3 0 1 1
* nofuelrod plane liqlev iaxcnd
  0 3 0 0
* nmwrx nfc1 nfc11 hdri hdro
  0 0 0 0.0 0.0
* nhot nodes fmno nzmax refflood
  0 4 0 3 0
* dtxht(1) dtxht(2) dznht hgapo
  0.0 0.0 100.0 4600.0

* idbcin * 0 0 0e
* idbcon * 2 2 2e
* qflxbc01 * 0.0e
* qflxbc01 * 0.0e
* qflxbc01 * 0.0e
* hcomon2 * 2 2 0 0e
* hcomon2 * 2 3 0 0e
* hcomon2 * 2 4 0 0e
* dhtstrz * 1.4 1.4 1.4e
* rdx * 49.0e
* radrd * 0.0 3.6347E-3 6.0579E-3 7.1501E-3e
* matrd * 1 1 2 e
```
* nfax *  1  1  1e
* rftn *  450.0  450.0  450.0  450.0s
* rftn *  450.0  450.0  450.0  450.0s
* rftn *  450.0  450.0  450.0  450.0e
* fpuo2 *  0.0e
* ftd *  1.0e
* gmix * f  0.0e
* gmles *  0.0e
* pgapt *  0.0e
* plvol *  0.0 e
* pslen *  0.0 e
* clenn *  0.0 e
* burn *  0.0  0.0  0.0e
*****************************************************************************
* Finished Heat Structure Section of Model *
*****************************************************************************

* Starting Power Components *
*****************************************************************************

****** type num userid component name
power 901 1 power data input test1
* numpwr chanpow 1 0
* htnum 4 e
* irpwty ndgx ndhx nrts nhist
  5 0 -11 5 0
* izpwtr izpwsv nzpwtb nzpwsv nzpwr
  0 1 1 0 0
* ipwrad ipwdep promheat decaheat wtbypass
  0 0 0.0 0.0 0.0 0.0
* nzpwz nzpwi nfbpwt nrpwr nrpwi
  0 0 0 0 0 0
* react tneut rpwoff rrpwmx rpwsc1
  0.0 0.0 0.0 1.0
* rpowri zpwin zpwoff rzpwmx
  4.3102E6 0.0 0.0
* extsou pldr pdrat fucrac
  0.0 0.0 1.3 0.7
* rdpwr 1.0 1.0 1.0s
* rdpwr 0.0e
* cpowr 1.0e
* zpwtbl* 1.0s
* zpwtbl* 1.0 1.0 1.0e
*****************************************************************************
* Finished Power Components *
*****************************************************************************
```
end
*
*****************
* Timestep Data *
*****************
*        dtmin         dtmax          tend         rtwfp
  1.0E-5           1.0        1000.0         100.0
*        edint         gfint        dmpint        sedint
      100.0          10.0          10.0          50.0
*
*      endflag
     -1.0

PARCS Input File

***************************************************************************
**
CASEID ss         Small Test Problem
***************************************************************************
**
CRTL
core_type  BWR
core_power  100.00000  ! Initial core power level in %
ppm        0.0       ! Initial boron concentration in ppm
!       bank1 (480-out,0-in)
! bank_pos  480.0
th_fdbk    T
xe_sm       3 0
! xe_sm      1 0
! 0 : no xe, 1 : eq. xe   2 : tr. xe  3 : given xe
decay_heat T
ROT_ADF     T
! for LPRM
pin_power  F
ext_th     T    ../maptab_1ch    TRAC    1    1
transient  F
restart    F   ss_1.rst   0
! input iteration planar    adj
! edit    table    power    pin    reac
print_opt  T    F    T    F    F
! fdbk flux planar
! rho precurs flux Xe T/H
print_opt  F    F    F    T    T
!! oneD   Radial    assy
!! const  Shape    const
! print_opt  F    F    F
!
! Jean LPRM
! oneD   PKRE   Radial    Radial    assy
! const  Data    Shape    Shape    const
print_opt  F    F    F    T    F
oned_kin  F    SA1D
PARAM !table 6
  n_iters 5 500
  conv_ss 1.0e-6 5.e-5 5.e-4 0.001 !keff, globfs, locfs, tempf
  wielandt 0.04 0.1 1.0
  nodal_kern HYBRID
  nlupd_ss 3 3 1
  nlupd_ss 100 100 100
  eps_anm 0.005
  eps_erf 0.005
  decusp 0
  init_guess 0

XSEC !table 7
  func_type 13 95
  dnp_ngrp 6
  kin_comp 1 1 -435
  pbtt specs
  dnp_beta 0.000167 0.001134 0.001022 0.002152 0.000837 0.000214
  dnp_lambda 0.012813 0.031536 0.124703 0.328273 1.405280 3.844728

GEOM !table 8
  file ../geom

TH !table 9
  !fix assume all assembles are 7x7, no guide/instrumentation tubes
  n_pingt 49 0 !npin, ngt
  !fix by Yunlin Xu: 3293/764 = 4.310209 3293*61.6459% = 2030MW
  FA POWPIT 4.31021 15.24 !assembly power (Mw) and pitch(cm)
  !
  pin_dim 5.0000 6.0000 0.900 6.0000 !pin radii, rs, rw, tw, and rgt in mm
  !fix: 555-273 = 282, 9585/764 = 12.548
  flow_cond 282.0 12.548 !tin, cmfrfa (Kg/sec)
  !
  pbtt spec
  CDC_DED 1 1
  !format: CDC_DED CDC_op DED_op
  ! CDC_op: integer for coolant density correction option:
  ! = 0 no correction (old models),
  ! = 1 correct with by pass density (PBTT)
  ! = 2 correct with bypass, and water rod densities (ESBWR)
  ! DED_op: integer for direct energy deposition option:
  ! = 0 one whole core factor for coolant (old models),
  ! = 1 two whole core factors for coolant, bypass (PBTT)
  ! = 2 three whole core factors for coolant, bypass, water rod (can be used in ESBWR)
  ! = 3 three node-wise coolant factors, bypass, water rod (ESBWR)
gamma_frac 0.02 0.017                !direct heating fraction
CDC_DAT 0.761 0.401
hgap 10000.                      !hgap(w/M^2-C)
n_ring 6                          !number of meshes in pellet
thmesh_x 1*1 !Number of T/H Nodes per FA in X-dir
thmesh_y 1*1 !Number of T/H Nodes per FA in Y-dir
thmesh_z 1 2 3 !junction locations
freeze_tf F 800.0
freeze_dm F 300.0
write_fbv T ss3d.fbv
read_dopl F ss3d.fbv
read_tmdm F ss3d.fbv

!********************************************************************
**********
!PFF table 10, power form function
PFF
npin_side 7
pff_comp 1 1 -435
pff_unrodd 1 !group 1 of set 1
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
pff_unrodd 2 !group 2 of set 1
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
pff_rodded 1 !group 1 of set 1
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
pff_rodded 2 !group 2 of set 1
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.

!********************************************************************
**********
!PLOT
! file sscoupl.plc
! file trcoupl.plc

**********
TRAN !table 11
time_step 5.0 0.00001
expo_opt F F
Scram F 95.0 0.0 143.
pin_freq 1 !control lprm freq too
theta 1.0 0.5 0.5
! The above values need checking
conv_tr  0.001
nlupd_tr  5 1 5 10
eps_xsec  0.01
rst_freq  1

PARCS Geometry File

geo_dim   1  1  3             !nasyx,nasyy,nz
Rad_Conf
!1
  2 !1

  grid_x      1*15.240
  neutmesh_x  1*1
  grid_y      1*15.240
  neutmesh_y  1*1
  grid_z      3*140.0
Boun_Cond  0  0  0  0  0  0     !ibcw,ibce,ibcn,ibcs,ibcb,ibct

planar_reg 1
  2
pr_assign  3*1
CR_axinfo  0.0    0.000    !fully inserted position and step size

bank_conf
  1
adf_rot
  0
det_z_loc 1 1
  1
det_xy_loc 1 0

det_name
  1       D_16-57

PARCS MAPTAB File

*  
%DOPL
AVG
    * LINC  0.7
*  
%REFLPROP
    565.0  565.0  764.0  0.0  0.0
*  tcoolrefl(K) tfuelrefl(K) rhomixrefl alparefl ppmrefl
%TRIP
    1
*  
* Volume to Node Table
*  
%TABLE1
B.3 14-Node Test Problem Representative of a BWR

TRACE Steady State Input File

free format
*
*
*************
* main data *
*************
*
* numtcr ieos inopt nmat id2o
  2 0 1 0 0
This is a test problem for my thesis. It represents a small BWR channel.
*
*
*
*****************
* namelist data *
*****************
*
&inopts
 cpuflg=1,
 itdmr=0,
 nosets=1,
 nsolver=1,
 usesjc=3,
 npower=1,
 nhtstr=1
 &end
*
*****************
* Model Flags *
*****************
*
* dstep timet
  0 0.0
* stdyst transi ncomp njun ipak
  1 0 5 2 1
* epso    epss
  1.0E-3  1.0E-10
* oitmax  sitmax  isolut  ncontr  nccfl
  10     10       0       0     0
* ntsv    ntcb    ntcf    ntrp    ntcp
  1   0        0       1     0
*
******************************
* component-number data *
******************************
* Component input order (IORDER)
**-- type ---- num ------------- name ----------------  +    jun1
jun2  jun3
* FILL     *      1 s * velocity bc                    +       1
* PIPE     *      2 s * subcooled liquid channel       +       1      3
* BREAK    *      3 s * pressure bc                    +       3
* HTSTR    *      4 s * powered-rod conductor         +
* POWER    *    901 e * power data input test1         +
*
****************************************************
* Starting Signal Variable Section of Model      *
****************************************************
*         idsv          isvn          ilcn          icn1          icn2
 1       0     0       0       0   0
****************************************************
* Finished Signal Variable Section of Model      *
****************************************************
*
****************************************************
* Starting Trip Section of Model  *
****************************************************
*         Trip Storage Count Card
*         ntse          ntct          ntsf          ntdp          ntsd
  0     0        0       0     0
*trip
*         idtp          isrt          iset          itst          idsg
  -2     2       0       1     1
*         setp(1)      setp(2)
  0.0    0.1
*         dtsp(1)      dtsp(2)
  0.0    0.0
*         ifsp(1)      ifsp(2)
  0     0
*
****************************************************
* Finished Trips: Starting Extras*
* Finished Trip Section of Model *

```
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</tbody>
</table>

<table>
<thead>
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<th>component name</th>
</tr>
</thead>
<tbody>
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</tbody>
</table>
```

** Remarks:**
- velocity bc
- subcooled liquid channel
- gravitational acceleration
- Reynolds number
- friction coefficient
- fluid dynamic viscosity
- fluid density
<table>
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<th>userid</th>
<th>component name</th>
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*** Starting Heat Structure Section of Model ***

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---

---

---
```
12 0 1 1
  * nofuelrod  plane  liqlev  iaxcnd
    0 3 0 0
  * nmwrx  nfcil  nfcil  hdri  hdro
    0 0 0.0 0.0
  * nhot  nodes  fmno  nzmax  reflood
    0 4 0 30 0
  * dtxht(1)  dtxht(2)  dznht  hgapo
    0.0 0.0 100.0 4600.0
  *
  * idbcin * 0 0 0 0s
  * idbcin * 0 0 0 0s
  * idbcin * 0 0 0 0e
  * idbcon * 2 2 2 2s
  * idbcon * 2 2 2 2s
  * idbcon * 2 2 2 2e
  * qflxbcol1 * 0.0e
  * qflxbcol1 * 0.0e
  * qflxbcol1 * 0.0e
  * qflxbcol1 * 0.0e
  * qflxbcol1 * 0.0e
  * qflxbcol1 * 0.0e
  * qflxbcol1 * 0.0e
  * hcomon2 * 2 2 0 0e
  * hcomon2 * 2 3 0 0e
  * hcomon2 * 2 4 0 0e
  * hcomon2 * 2 5 0 0e
  * hcomon2 * 2 6 0 0e
  * hcomon2 * 2 7 0 0e
  * hcomon2 * 2 8 0 0e
  * hcomon2 * 2 9 0 0e
  * hcomon2 * 2 10 0 0e
  * hcomon2 * 2 11 0 0e
  * hcomon2 * 2 12 0 0e
  * hcomon2 * 2 13 0 0e
  * dhtstrz * 0.35 0.35 0.35 0.35s
  * dhtstrz * 0.35 0.35 0.35 0.35s
  * dhtstrz * 0.35 0.35 0.35 0.35s
  * rdx * 49.0e
  * radrd * 0.0 3.6347E-3 6.0579E-3 7.1501E-3e
  * matrd * 1 1 2 e
  * nfax * 1 1 1 1s
  * nfax * 1 1 1 1s
  * nfax * 1 1 1 1e
  * rftn * 450.0 450.0 450.0 450.0s
  * rftn * 450.0 450.0 450.0 450.0s
  * rftn * 450.0 450.0 450.0 450.0s
  * rftn * 450.0 450.0 450.0 450.0s
  * rftn * 450.0 450.0 450.0 450.0s
```
* rftn * 450.0 450.0 450.0 450.0s
* rftn * 450.0 450.0 450.0 450.0s
* rftn * 450.0 450.0 450.0 450.0s
* rftn * 450.0 450.0 450.0 450.0s
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* rftn * 450.0 450.0 450.0 450.0s
* rftn * 450.0 450.0 450.0 450.0s
* rftn * 450.0 450.0 450.0 450.0s
* fpuo2 * 0.0e
* ftd * 1.0e
* gmix * f 0.0e
* gmixes * 0.0e
* pgapt * 0.0e
* plvol * 0.0 e
* pslen * 0.0 e
* clemn * 0.0 e
* burn * 0.0 0.0 0.0 0.0s
* burn * 0.0 0.0 0.0 0.0s
* burn * 0.0 0.0 0.0 0.0e
********************************************************************************
* Finished Heat Structure Section of Model *
********************************************************************************

****************************************************
* Starting Power Components *
****************************************************

**** type num userid component name
power 901 1 power data input test1
* numpwr chanpow 1 0
* htsnum 4 e
* irpwty ndgx ndhx nrts nhist
  5 0 0 5 0
* izpwtr izpwsv nzpwtb nzpwsy nzpwrf
  0 1 1 0 0
* ipwrad ipwdep promheat decaheat wtbypass
  0 0 0.0 0.0 0.0
* nzpwz nzpwi nfbpwt nrpwr nrpwi
  0 0 0 1 0
* react tneut rpowoff rrpwmx rpwsc1
  0.0 0.0 0.0 0.0 1.0
* rpowri zpwin zpwoff rzpwmx
  4.3102E6 0.0 0.0 0.0 1.0
* extsou pldr pdrat fucrac
  0.0 0.0 1.3 0.7
* rdppwr 1.0 1.0 1.0 0.0e
* cpowr 1.0e
* zpwtbl* 1.0s
* zpwtbl* 1.0 1.0 1.0 1.0 1.0s
* zpwtbl* 1.0 1.0 1.0 1.0 1.0s
* zpwtbl* 1.0 1.0 1.0e
PARCS Input File

!********************************************************************
**********
CASEID ss Small Test Problem
!********************************************************************
**********
CNTL

core_type  BWR
core_power 100.00000 ! Initial core power level in %
ppm 0.0 ! Initial boron concentration in ppm
! bank1 (480-out,0-in)
bank_pos 480.0
th_fdbk  T
xe_sm 3 0
! xe_sm 1 0
! 0 : no xe, 1 : eq. xe 2 : tr. xe 3 : given xe
decay_heat  T
ROT_ADF  T
! for LPRM
pin_power  F
ext_th  T ../maptab_1ch  TRAC  1  1
transient  F
restart  F ss_1.rst  0
! input  iteration  planar  adj
! edit  table  power  pin  reac
print_opt  T  F  T  F  F
! fdbk  flux  planar
! rho  precurs  flux  Xe  T/H
print_opt  F  F  F
!! oneD  Radial  assy
!! const  Shape  const
! print_opt  F  F  F

1.0E-5  1.0  1000.0  100.0
*        edint         gfint        dmpint        sedint
        100.0  10.0  10.0  50.0
PARAM !table 6
n_iters    5      500
conv_ss    1.0e-6 5.e-5 5.e-4 0.001 !keff,globfs,locfs,tempf
wielandt   0.04 0.1 1.0
nodal_kern HYBRID
nlupd_ss   3 3 1
! nlupd_ss   100 100 100
eps_anm    0.005
eps_erf    0.005
decusp     0
init_guess 0
!********************************************************************
**********
XSEC !tabl 7
func_type  13 95
dnp_ngrp   6
kin_comp   1 1 -435
! pbtt specs
dnp_beta   0.000167 0.001134 0.001022 0.002152 0.000837 0.000214
dnp_lambda 0.012813 0.031536 0.124703 0.328273 1.405280 3.844728
!********************************************************************
**********
GEOM !table 8
file ../geom
!********************************************************************
**********
TH !table 9
!fix assume all assembiles are 7x7, no guide/instrumentation tubes
n_pingt    49 0 !npin,ngt
!fix by Yunlin Xu: 3293/764=4.310209     3293*61.6459% = 2030MW
FA_POWPIT  4.31021 15.24 !assembly power(Mw) and pitch(cm)
!
pin_dim    5.0000 6.0000 0.900 6.0000 !pin radii, rs,rw,tw, and rgt in mm
!fix: 555-273=282, 9585/764=12.548
flow_cond  282.0 12.548 !tin,cmfrfa(Kg/sec)
!
! pbtt spec
CDC_DED    1 1
!format: CDC_DED   CDC_op     DED_op
! CDC_op: integer for coolant density correction option:
! =0 no correction(old models),
! =1 correct with by pass density(PBTT)
! =2 correct with bypass, and water rod densities(ESBWR)
! DED_op: integer for direct energy deposition:option:
= 0 one whole core factor for coolant (old models),
= 1 two whole core factors for coolant, bypass (PBTT)
= 2 three whole core factors for coolant, bypass, water rod (can be used in ESBWR)
= 3 three node-wise coolant factors, bypass, water rod (ESBWR)

!direct heating fraction
gamma_frac 0.02 0.017
CDC_DAT 0.761 0.401
hgap 10000.

!number of meshes in pellet
n_ring 6
thmesh_x 1*1
in X-dir
thmesh_y 1*1
in Y-dir
thmesh_z 1 2 3 4 5 6 7 8 9 10 11 12 13 14

!junction locations
freeze_tf F 800.0
freeze_dm F 300.0
write_fbv T ss3d.fbv
read_dopl F ss3d.fbv
read_tmdm F ss3d.fbv

!********************************************************************
**********
!PFF  table 10, power form function
PFF
npin_side 7
pff_comp 1  1 -435
pff_unrodd 1  !group 1 of set 1
  1. 1. 1. 1.
  1. 1. 1. 1.
  1. 1. 1. 1.
  1. 1. 1. 1.
pff_unrodd 2  !group 2 of set 1
  1. 1. 1. 1.
  1. 1. 1. 1.
  1. 1. 1. 1.
  1. 1. 1. 1.
pff_rodded 1  !group 1 of set 1
  1. 1. 1. 1.
  1. 1. 1. 1.
  1. 1. 1. 1.
  1. 1. 1. 1.
pff_rodded 2  !group 2 of set 1
  1. 1. 1. 1.
  1. 1. 1. 1.
  1. 1. 1. 1.
  1. 1. 1. 1.

!********************************************************************
**********
!PLOT
! file sscoupl.plc
! file trcoupl.plc

tran !table 11
time_step  5.0 0.00001
expo_opt  F  F
Scram     F 95.0 0.0 143.  !control lprm freq too
pin_freq  1

! The above values need checking
theta    1.0  0.5  0.5
conv_tr  0.001
nlupd_tr 5 1 5 10
eps_xsec 0.01
rst_freq 1

PARCS Geometry File

geo_dim   1 1 14  !nasyx,nasyy,nz
Rad_Conf
!1
  2 !1
grid_x    1*15.240
neutmesh_x 1*1
grid_y    1*15.240
neutmesh_y 1*1
grid_z    14*35.0
Boun_Cond 0 0 0 0 1 1  !ibcw,ibce,ibcn,ibcs,ibcb,ibct
planar_reg 1
  433
planar_reg 2
 25
pr_assign  1 12*2 1
CR_axinfo  0.0  0.000  !fully inserted position and step size
bank_conf
  1
adf_rot
  0
det_z_loc 1 1
  1
det_xy_loc 1
  0
det_name
  1       D_16-57

PARCS MAPTAB File

*  
%DOPL  
AVG  
* LINC  0.7
*  
%REFLPROP
  565.0  565.0  764.0  0.0  0.0
* tcoolrefl(K) tfuelrefl(K) rhomixrefl alparefl ppmrefl
B.4 14-Node Test Problem Representative of a PWR

TRACE Steady State Input File
free format
*
*************
* main data *
*************
*
* numtcr  ieos  inopt  nmat  id2o
This is a test problem for my thesis. It represents a small BWR channel.

*****************
* namelist data *
*****************

&inopts
  cpuflg=1,
  itdmr=0,
  nsolver=1,
  usesjc=3,
  npower=1,
  nhtstr=1
&end

*****************
* Model Flags *
*****************

*      dstep         timet
0           0.0
*      stdyst         transi         ncomp         njun         ipak
1           0           5           2           1
*      epso         epss
1.0E-3       1.0E-10
*      oitmax         sitmax         isolut         ncontr         nccfl
10            10             0             0             0
*      ntsv         ntcb         ntcf         ntrp         ntcp
2           0           0           2           0

**************************************************
* Component-number data *
**************************************************

* Component input order (IORDER)
--- type ---- num -------------- name -------------- +    jun1
jun2    jun3
  FILL   * 1 s * velocity bc +  1
  PIPE   * 2 s * subcooled liquid channel +  1  3
  BREAK  * 3 s * pressure bc +  3
  HTSTR  * 4 s * powered-rod conductor +
  POWER  * 901 e * power data input test1 +

**************************************************
* Starting Signal Variable Section of Model *
**************************************************

*      idsv         isvn         ilcn         icn1         icn2
1           0           0           0           0
*       idsv       isvn       ilcn       icn1       icn2
54 18 901 0 0

********************************************************************
* Finished Signal Variable Section of Model                      *
********************************************************************

********************************************************************
* Starting Trip Section of Model                               *
********************************************************************

*       Trip Storage Count Card
*               ntse       ntct       ntsf       ntdp       ntsd
*                          0       0       0       0       0

*trip
  *       idtp       isrt       iset       itst       idsg
  -2  2  0  1  1

  *       setp(1)       setp(2)
  0.0  0.1

  *       dtsp(1)       dtsp(2)
  0.0  0.0

  *       ifsp(1)       ifsp(2)
  0  0

*d: Reactor trip on High Flux
*trip  112
  *       idtp       isrt       iset       itst       idsg
  112  2  0  1  54

  *       setp(1)       setp(2)
  0.0  2.0E7

  *       dtsp(1)       dtsp(2)
  0.4  0.4

  *       ifsp(1)       ifsp(2)
  0  0

********************************************************************
* Finished Trips: Starting Extras                                *
********************************************************************

********************************************************************
* Finished Trip Section of Model                               *
********************************************************************

*******   type       num       userid       component name
fill                       1       1       velocity bc
  *       junl       ifty       ioff
  1       1       0
* twtold  rfmx  concin  felv
  0.0  0.0  0.0  0.0
* dxin  volin  alpin  vlin  tlin
  0.2976  0.0577  0.0  4.9587  562.0
* pin  pain  flowin  vvin  tvin
  1.58E7  0.0  0.0  0.0  562.0

******
type  num  userid  component name
pipe  2  1  subcooled liquid channel
* ncells  nodes  jun1  jun2  epsw
  14  0  1  3  0.0
* nsides
  0
*  ichf  icnc  pipetype  ipow  npipes
  1  0  0  0  0  1
* radin  th  houtl  houtv  toutl
  0.0  0.0  0.0  0.0  0.0
* toutv  pwin  pwoff  rpwmx  pwsc1
  0.0  0.0  0.0  0.0  0.0
* dx  *
  0.2976  0.2976  0.2976  0.2976  0.2976
* dx  *
  0.2976  0.2976  0.2976  0.2976  0.2976
* dx  *
  0.2976  0.2976e
* vol  *
  0.0577  0.0577  0.0577  0.0577  0.0577s
* vol  *
  0.0577  0.0577  0.0577  0.0577  0.0577s
* vol  *
  0.0577  0.0577  0.0577  0.0577  0.0577s
* vol  *
  0.0577  0.0577e
* fa  *
  0.19385081  0.19385081  0.19385081  0.19385081  0.19385081s
* fa  *
  0.19385081  0.19385081  0.19385081  0.19385081  0.19385081s
* fa  *
  0.19385081  0.19385081  0.19385081  0.19385081  0.19385081s
* fa  *
  0.19385081  0.19385081  0.19385081  0.19385081  0.19385081e
* fric  *
  0.0  0.0  0.0  0.0  0.0s
* fric  *
  0.0  0.0  0.0  0.0  0.0s
* fric  *
  0.0  0.0  0.0  0.0  0.0s
* fric  *
  0.0  0.0  0.0e
* grav  *
  1.0  1.0  1.0  1.0  1.0s
* grav  *
  1.0  1.0  1.0  1.0  1.0s
* grav  *
  1.0  1.0  1.0  1.0e
* grav  *
  1.0  1.0  1.0e
* hd  *
  0.1305  0.1305  0.1305  0.1305  0.1305s
* hd  *
  0.1305  0.1305  0.1305  0.1305  0.1305s
* hd  *
  0.1305  0.1305  0.1305  0.1305  0.1305s
* hd  *
  0.1305  0.1305  0.1305e
* nff  *
  0  0  0  0s
* nff  *
  0  0  0  0s
* nff  *
  0  0  0  0s
* nff  *
  0  0  0e
* alp  *
  0.0  0.0  0.0  0.0s
* alp  *
  0.0  0.0  0.0  0.0s
* alp  *
  0.0  0.0  0.0  0.0s
* alp  *
  0.0  0.0e
* vl  *
  5.0  5.0  5.0  5.0s
* vl  *
  5.0  5.0  5.0  5.0s
* vl    * 5.0  5.0  5.0  5.0  5.0s
* vl    * 5.0  5.0  5.0  5.0  5.0e
* vv    * 0.0  0.0  0.0  0.0  0.0s
* vv    * 0.0  0.0  0.0  0.0  0.0s
* vv    * 0.0  0.0  0.0  0.0  0.0s
* vv    * 0.0  0.0  0.0  0.0e
* tl    * 564.0  564.0  564.0  564.0  564.0s
* tl    * 564.0  564.0  564.0  564.0  564.0s
* tl    * 564.0  564.0  564.0  564.0  564.0s
* tl    * 564.0  564.0e
* tv    * 564.0  564.0  564.0  564.0  564.0s
* tv    * 564.0  564.0  564.0  564.0  564.0s
* tv    * 564.0  564.0  564.0  564.0  564.0s
* tv    * 564.0  564.0e
* p     * 1.58E7  1.58E7  1.58E7  1.58E7  1.58E7s
* p     * 1.58E7  1.58E7  1.58E7  1.58E7  1.58E7s
* p     * 1.58E7  1.58E7  1.58E7  1.58E7  1.58E7s
* p     * 1.58E7  1.58E7  1.58E7e
* pa    * 0.0  0.0  0.0  0.0  0.0s
* pa    * 0.0  0.0  0.0  0.0  0.0s
* pa    * 0.0  0.0  0.0  0.0  0.0s
* pa    * 0.0  0.0  0.0e

****** type num userid component name
break  3  1 pressure bc
* jun1 ibty isat ioff adjpress
  3  0  0  0  0
* dxin volin alpin tin pin
  0.2976  0.0577  0.0  600.0 1.58E7
* pain concin rbmx poff belv
  0.0  0.0  0.0  0.0  0.0

********************************************
* Starting Heat Structure Section of Model *
********************************************

****** type num userid component name
htstr  4  0 powered-rod conductor
* nzhstr ittc hscyl ichf
  12  0  1  1
* nofuelrod plane liqlev iaxcnd
  0  3  0  0
* nmwrx nfcil nfcil hdri hdro
  0  0  0  0.0  0.0
* nhot nodes fmno nzmax reflood
  0  4  0  30  0
* dtxht(1) dtxht(2) dznht hgapo
  0.0  0.0  100.0 4600.0
* idbcin * 0  0  0  0s
* idbcin * 0  0  0  0s
* idbcin * 0  0  0  0e
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* pslen * 0.0 e
* clenn * 0.0 e
* burn * 0.0 0.0 0.0 0.0 0.0s
* burn * 0.0 0.0 0.0 0.0 0.0s
* burn * 0.0 0.0 0.0 0.0 0.0e

********************************************
* Finished Heat Structure Section of Model *
********************************************

****** type num userid component name
power 901 1 power data input test1
* numpwr chanpow 1 0
* htnum * 4 e
* irpwt type ndgx ndhx nrts nhist
  5 0 0 5 0
* izpwt type izpwsv nzpwtb nzpwsv nzpwrf
  0 1 1 0 0
* ipwrad type ipwdep promheat decaheat wtbypass
  0 0 0 0 0
* nzpwl type nzpwi nfbpwt nrpwr nrpwi
  0 0 1 0 0
* react type tneut rpwoff rpwmx rpwsc1
  0.0 0.0 0.0 1.0
* rpowr * 1.0 1.0 1.0 0.0e
* cpowr * 1.0e
* zpwt1 * 1.0s
* zpwt1* 1.0 1.0 1.0 1.0 1.0s
* zpwt1* 1.0 1.0 1.0 1.0 1.0s
* zpwt1* 1.0 1.0e

********************************************
* Finished Power Components *
********************************************

end

*****************
* Timestep Data *
*****************
* dtmin dtmax tend rtwfp
  1.0E-6 1.0 1000.0 100.0
PARCS Input File

!********************************************************************
**********
CASEID ss         Small Test Problem
!********************************************************************
**********

CNTL

core_power 100.00000  ! Initial core power level in %
bank_pos  971.0
th_fdbk   T
decay_heat T
ROT_ADF   T
pin_power F
ext_th   T ../maptab_1ch TRAC l l
transient F
restart F ss_1.rst 0
!
! input iteration planar adj
! edit table power pin reac
print_opt   T F T F F
!
! fdbk flux planar
! rho precurs flux Xe T/H
print_opt   F F F F F
!
! oneD PKRE Radial Radial assy
! const Data Shape Shape const
print_opt   F F F T F
oned_kin   F SA1D
!
!********************************************************************
**********
PARAM

conv_ss   1.e-6 5.e-5 1.e-3 0.001 !epseig,eps12,eps1inf,eps1f
eps_erf   0.010
eps_anm   0.000001
nlupd_ss  5 5 1
init_guess 0
!

!********************************************************************
**********
XSEC

func_type  11
dnpngrp  6
dhp_beta 2.35402E-02 1.89077E-02 1.39236E-02 6.90315E-03
3.56888E-03 3.31633E-03

dhp_lambda 1.05345E-01 8.37149E-03 5.20337E-04 4.73479E-05
3.28153E-06 1.17537E-11
kin_comp   1 1 -438

*        edint         gfint        dmpint        sedint
100.0  1.0E-4  10.0  50.0
*
*        endflag
-1.0
dnp_beta  0.000153  0.001086  0.000965  0.002019  0.000791  0.000197
dnp_lambda  0.012818  0.031430  0.125062  0.329776  1.414748  3.822362
neut_velo  1.83E7  4.01E5

!********************************************************************
**********
GEOM  !table 8
file  ../geom
!********************************************************************
**********
TH
n_pingt  208 17  !npin,ngt
fa_powpit  15.661 21.811  !assembly power(Mw) and
pitch(cm)  
pin_dim  4.6955 5.4640 0.673 6.731  !pin radii, rs,rw,tw, and
rgt in mm
flow_cond  289.84 90.7448  !tin,cmfrfa(Kg/sec)
gamma_frac 0.0  !direc heating fraction
hgap  11356.  !hgap(w/M^2-C)
n_ring  6  !number of meshes in pellet
thmesh_x  1*1  !Number of T/H Nodes per FA
in X-dir
thmesh_y  1*1  !Number of T/H Nodes per FA
in Y-dir
thmesh_z  1 2 3 4 5 6 7 8 9 10 11 12 13 14  !junction locations
!********************************************************************
**********
PFF  table 10, power form function
PFF
npin_side  7
pff_comp  1 -435
pff_unrodd  1  !group 1 of set 1
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
pff_unrodd  2  !group 2 of set 1
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
pff_rodded  1  !group 1 of set 1
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
pff_rodded  2  !group 2 of set 1
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
1. 1. 1. 1.
!********************************************************************
**********
!PLOT
!    file sscoupl.plc
!    file trcoupl.plc

**********
**
TRAN
    Time_Step  100.0 0.1 100.0 10.0
    Scram    T 114.0 0.4 2.2
    nlupd_tr 5 1 5 10
    conv_tr  0.001
    eps_xsec 0.001
.

PARCS Geometry File

geo_dim  1 1 14            !nasyx,nasyy,nz
Rad_Conf
!1
  !
  grid_x  1*21.810
  neutmesh_x 1*1
  grid_y  1*21.810
  neutmesh_y 1*1
  grid_z  14*29.76
Boun_Cond  0  0  0  0  1  1     !ibcw,ibce,ibcn,ibcs,ibcb,ibct
planar_reg 1
  26
planar_reg 2
  100
pr_assign  1 12*2 1
! CR_axinfo 36.2255 0.3531   !fully inserted position and step size
CR_axinfo 170.2255 1.0000   !fully inserted position and step size
bank_conf
  1

PARCS MAPTAB File
*
%DOPL
AVG
*  LINC  0.7
*
%REFLPROP
  565.0  565.0  764.0  0.0  0.0
*  tcoolrefl(K) tfuelrefl(K) rhomixrefl alparefl ppmrefl
%TRIP
  112
*
* Volume to Node Table
*
%TABLE1

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| 2 | 2 | 0 | 2 | 1.0000
| 2 | 3 | 0 | 3 | 1.0000
| 2 | 4 | 0 | 4 | 1.0000
| 2 | 5 | 0 | 5 | 1.0000
| 2 | 6 | 0 | 6 | 1.0000
| 2 | 7 | 0 | 7 | 1.0000
| 2 | 8 | 0 | 8 | 1.0000
| 2 | 9 | 0 | 9 | 1.0000
| 2 |10 | 0 |10 | 1.0000
| 2 |11 | 0 |11 | 1.0000
| 2 |12 | 0 |12 | 1.0000
| 2 |13 | 0 |13 | 1.0000
| 2 |14 | 0 |14 | 1.0000

* Heat Structure to Node Table *

%TABLE2

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| 4 | 1 | 2 | 3 | 1.0000
| 4 | 1 | 3 | 4 | 1.0000
| 4 | 1 | 4 | 5 | 1.0000
| 4 | 1 | 5 | 6 | 1.0000
| 4 | 1 | 6 | 7 | 1.0000
| 4 | 1 | 7 | 8 | 1.0000
| 4 | 1 | 8 | 9 | 1.0000
| 4 | 1 | 9 |10 | 1.0000
| 4 | 1 |10 |11 | 1.0000
| 4 | 1 |11 |12 | 1.0000
| 4 | 1 |12 |13 | 1.0000
| 4 | 1 |12 |14 | 0.0000
Justin Kyle Watson was born January 15, 1972 in Chambersburg, Pennsylvania. He graduated Chambersburg Area Senior High School in 1990. He received his Bachelors degree in Nuclear Engineering from the Pennsylvania State University in 1996. He then entered graduate school and received a Master in Nuclear Engineering from the Pennsylvania State University in 2001. During this time period he developed and interest in high performance computing for scientific applications. In 2001 he accepted a position as Senior Applications Analyst Programmer at the Applied Research Laboratory at Pennstate University where he built and maintained the hardware and software for several beowulf clusters. In late 2004 he took a Research Faculty position at the Applied Research Laboratory where he worked on government research projects. He primarily worked as a code developer for the next generation nuclear reactor safety analysis code for the Nuclear Regulatory Commission. He has also taught a senior level elective course in Nuclear Engineering titled Power Plant Simulation. His current research interest are in the area of coupled multi-physics simulations of core physics and computational fluid mechanics.