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Simulation of Counterintuitive Pressure Drop in a Parallel Flow Design for a Specimen Basket for Use in the Advanced Test Reactor

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SIMULATION OF COUNTERINTUITIVE PRESSURE DROP IN A PARALLEL
FLOW DESIGN FOR A SPECIMEN BASKET FOR USE IN THE ADVANCED
TEST REACTOR

by

Adam X. Zabriskie

A thesis submitted in partial fulfillment
of the requirements for the degree
of
MASTER OF SCIENCE
in
Mechanical Engineering

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2012
Abstract

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Adam X. Zabriskie, Master of Science
Utah State University, 2012

Major Professor: Dr. Heng Ban
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The Boosted Fast Flux Loop (BFFL) will expand the Advanced Test Reactor (ATR) at Idaho National Laboratory. Part of the BFFL is a new corrosion test cap section for testing in the ATR. The corrosion test cap section was designed with parallel channels to reduce the pressure drop and allow coolant contact with specimens. The fluid experiment conducted by Idaho State University found the pressure drop not characteristic of parallel channel flow but greater than without parallel channels. A Computation Fluid Dynamics simulation using STAR-CCM+ was conducted with the objectives of showing sufficient flow through the test cap section for a corrosion test, verifying the fluid experiment’s validity, and explaining the abnormal pressure drop. The simulation used a polyhedral volume mesh and the k-ε turbulent model with segregated equations. Convergence depended on a low continuity residual and an unchanging pressure drop result. The simulation showed the same pattern as the fluid experiment. The simulation provided evidence of flow through the test cap section needed for a corrosion test. The specimen holding assembly was found to be a small contributor to the pressure drop. The counterintuitive pressure drop was found to be the sum of many factors produced from the geometry of the test cap section. The inlet of the test cap section behaved as a diverging nozzle before a sudden expansion into
the test cap section chamber with both creating a pressure drop. The chaotic flow inside
the chamber gave rise to pressure loss from mixing. The fluid exited the chamber through a
sudden contraction to a converging nozzle behaving exit, again, producing a pressure drop.
By varying the flow rate in the simulation, a disturbance in the flow where the gap fluid
separated into the parallel channels was found at high flow rates. At low flow rates the
pressure drop anomaly was not found. The corrosion test cap section could be used in the
ATR but with a higher pressure drop than desirable. The design of the corrosion test cap
section created the abnormal pressure drop.
Public Abstract

Simulation of Counterintuitive Pressure Drop in a Parallel Flow Design for a Specimen Basket for Use in the Advanced Test Reactor

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To continue improving nuclear energy, new materials must be tested in testing reactors such as the Advanced Test Reactor (ATR) at Idaho National Laboratory. A new test cap section allowed coolant to contact specimens tested in the ATR. A parallel channel test cap section should reduce the pressure drop across this section compared to a single channel. A fluid experiment conducted by Idaho State University showed the pressure drop was actually greater. A Computation Fluid Dynamics simulation using STAR-CCM+ was conducted of the fluid experiment to explain the abnormal pressure drop. The simulation provided evidence of flow through the test section required for a corrosion test and supported the results of the fluid experiment. Some pressure drop was caused by nozzle-like design and sudden expansion and contraction. Chaotic mixing produced some pressure drop. Flow disturbance related to flow rate caused a pressure drop at high flow rates when the fluid separated into each channel. The anomalous pressure drop was caused by the design of the test cap section.
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Chapter 1

Introduction

As energy needs continue to rise across the world, solutions to this demand must be found. Nuclear energy is one such solution, which is both reliable and available in quantity. New technology and research has improved nuclear energy since its discovery and continues to improve safety, efficiency, reliability, environmental impact, and sustainability. Nuclear energy will be used in the future and must be improved.

Material testing has greatly improved the nuclear energy field through improved materials and safety. The unique environment inside a nuclear reactor changes material properties. These changes are difficult to predict making in reactor experiments necessary to determine the changes and damage to materials. This behavior is largely dependent on the flux and energy levels of released nuclear radiation during fission. One type of radiation of particular importance is the bombardment damage from neutrons. The speed of a neutron is related to the energy of the neutron. Low energy neutrons, called thermal neutrons, damage materials differently than high energy neutrons, called fast neutrons. Which neutron type is present and damaging the material depends on the design of the reactor and the coolant used. The important thing is that both types of neutrons can weaken or change materials in such a way to cause early failure.

To avoid failure and damage, materials are first tested inside a nuclear reactor designed for this purpose. The Advanced Test Reactor (ATR) is a thermal neutron reactor designed and built for the testing of materials under radiation bombardment. The tested material specimen is placed inside the reactor and exposed to higher than normal doses of radiation. High doses of radiation allow for materials to be tested as if in a full life cycle inside a normal reactor, but only in a fraction of the time inside the ATR. The ATR has proven to be a valuable tool in the study of radiation damage and the behavior of materials and new
nuclear fuels under a thermal neutron reactor's radiation bombardment.

1.1 Material Damage from Neutrons

The way neutrons interact with material has already been studied so a brief overview will be given here. Neutron behavior in material is interesting due to the fact that neutrons have a neutral charge and are particles with mass. The neutron interacts with the nuclei of the atoms in the material. Because the nucleus of an atom is rather small compared to the total size of the atom, neutrons penetrate materials much like gamma or x-ray waves. Statistical methods are largely used to design shields and materials.

Neutrons interact with nuclei by colliding with them physically since neutrons carry no charge. Neutron collisions can occur as elastic, inelastic, or absorption collisions. Elastic collisions with the nucleus transfer kinetic energy to the atom. Elastic collisions behave much the same way as colliding billiard balls of differing mass. This is a major cause of damage to the crystal structure in metal material as neutrons physically knock atoms out of their original structure. Neutrons usually make several elastic collisions before their energy level has been reduced from fast to thermal. Each nucleus the neutron bounces off of takes some of the energy of the neutron. Elastic scattering could even turn a neutron around and send it out of the material. The geometry of the material can also funnel neutrons towards one area creating high damage areas.

Inelastic collisions are where the nucleus can absorb the energy of the colliding neutron without absorbing the neutron itself. This large transfer of energy causes the nucleus to release a gamma ray to return to a comfortable energy state. The resulting gamma ray can also cause damage if it has high energy. An inelastic neutron collision mostly slows down the neutron reducing the fast neutron to a thermal neutron.

A collision resulting in the capture of a neutron inside the nucleus of an atom is an absorption collision. Absorption collisions are more common when a neutron has been reduced to a thermal energy level. The additional neutron from the absorption collision changes the isotope of the atom it collided with. The new isotope could be unstable or not. An unstable isotope will become radioactive and decay. This new radiation could damage
the material. The product from the decay of the unstable isotope could introduce weakening impurities in the material as well. The creation of an isotope, stable or unstable from an absorption collision could change the cross sectional area. Even a created isotope could absorb another neutron from an absorption collision creating yet another isotope. This process could eventually change a stable isotope into a unstable radioactive isotope.

The probability of colliding with an atom is denoted by the materials cross section which is determined empirically from experimentation. The cross section is related to the size of the nucleus. The interaction of neutrons with the nucleus does not depend solely on the cross sectional area of the atom alone as stated in [1]. Certain energy levels of neutrons provide higher collisions with certain atoms. This explains why the thermal absorption cross section for one atom is different than the fast absorption cross section. The same dependency on the energy level of the neutron is true for the other types of cross sections for differing types of collisions. The cross sectional area depends, as reminded in [2], on the actual nucleus present, since even isotopes of the same element can have different cross sections.

This cross sectional area can be thought of as the statistical probability for a collision to happen. The larger the cross sectional area means a higher probability of collision. Because of this statistical probability, neutron damage can occur fairly deep into a material. The damage can also cluster around areas of high collision probabilities, thus making the geometry and orientation of the material important. Empirical data of cross sectional area compared to neutron energy level is needed to properly compute neutron penetration and collision behavior in materials used inside reactors.

Neutron bombardment of a material always produces one very dangerous change to the material. The material becomes activated and produces radiation when the neutrons are absorbed. Isotopes with relatively short half-life can introduce impurities into the metal in the form of new atoms not present before. These new impurities can not only change the properties of the material, but also change how the neutrons behave in the material and the radioactivity of the material. This type of damage is from absorption making it more common at a thermal neutron flux.
As [1] reminds, with all the energy the material receives from the interaction with the neutron collisions, the material is subject to thermal stress and strain. Thermal damage in the material depends largely on the material properties, the neutron flux, and the method of cooling. Non-uniform heating by neutron interactions can cause serious stresses which could cause the material to fail. Non-uniform heating could be caused by the location in the reactor or by damage changing the neutronics of the material. Thermal energy would cause impurities to migrate faster inside of a material and change the properties faster than if no thermal energy was present.

Fast neutrons have the speed or kinetic energy to displace atoms in materials. Thermal neutrons can also displace atoms as reported in [3]. The absorption of the thermal neutron was accompanied by a release of a gamma ray. The recoil from the emitting gamma ray could displace the atom. This type of damage was reported to be more significant in materials with a high thermal absorption cross section than fast neutron scattering cross section. The displaced atom leaves behind a vacancy in the lattice and becomes an interstitial atom.

Both [1] and [2] discuss the formation of interstitial atoms in a material from neutron collisions. The formation of interstitial atoms and the vacancy left in the lattice change the physical properties which depend on the lattice structure. The damaged lattice introduces stress and strains which can deform, weaken, and distort the material. The damaged lattice also stores the extra energy which can release more heat energy during a recovery process such as annealing. It is difficult to distinguish between the causes, fast or thermal neutron, of this type of damage since the resulting interstitial atom could have come from either.

Neutron bombardment can also increase the corrosion rate in basically two ways. Either the coolant can be altered to form compounds which can corrode materials or the material will be altered to become chemically reactive to another material or with the coolant. Crud formed from corrosion products can also deposit on surfaces and foul up the proper flow of fluid or transfer of heat between materials and coolant. This is a big concern in a reactor environment. Foreign material in the coolant and fouling could impair proper reactor operation or create an unsafe operating reactor.
1.2 Expanding the Advanced Test Reactor

Current efforts are underway to expand the ATR’s testing abilities for material damage. Tests for a fast neutron environment cannot be done inside a thermal neutron reactor. Even though fast neutrons are present in the reactor in small numbers, the large numbers of thermal neutrons would change the results of material testing. Damage from thermal neutrons would be included in the material along with fast neutron damage. There would be no way to separate or classify the two types of damage in a material being tested. Only by controlling the fast flux to thermal flux ratio can damage be classified as being from fast or thermal neutrons. Building an entirely new reactor just for a fast neutron environment, giving only fast neutron damage, would be costly if an alternative method could be just as effective and cheaper to modify an already existing test reactor.

The alternative method proposed in [4], named the Boosted Fast Flux Loop (BFFL), is in part to create a shielding screen of hafnium, which has a high thermal absorption cross sectional area, to allow only the fast neutrons to pass through and interact with the specimen of material being tested. A fast neutron environment with a much reduced, if not eliminated, thermal neutron flux would then exist inside of the hafnium shielding. The hafnium shielding would enclose the specimens for fast flux bombardment inside the ATR’s thermal reactor producing fast neutron damage to the specimen. ATR could then be used to study material behavior outside of the thermal neutron damage spectrum. This would expand the current capabilities of the reactor using these specimen shields in the BFFL.

Before this hafnium aluminide composite shield can be used, the effects of the thermal neutron environment on the material properties must be known for the shield itself. The shielding material is a hafnium and aluminum composite inside an aluminum matrix with varying amounts of hafnium being tested. A higher hafnium content will provide a lower thermal flux inside the shield. Since this new composite material will also be in contact with the coolant in the ATR, an experiment in the reactor must also test corrosion resistance while in the thermal neutron environment. Hafnium and aluminum are well known materials for use in nuclear reactors.
1.3 Hafnium

The choice to use hafnium as the primary material for shielding the specimens from thermal neutrons is normal. Hafnium has historically been used as a thermal neutron absorber. The ATR uses hafnium control rods to control the nuclear reaction. The thermal neutron capture cross section for hafnium was roughly $10200 \pm 5\% \text{ fm}^2 \ (102 \pm 5\% \text{ b})$ reported in [5]. Contrast this large value with the fast neutron capture cross sections from [6] which are in a range of about 700 to 1600 fm$^2$. The trend from [6] also suggests the capture cross section decreases as neutron energy increases, with certain energy levels producing high resonant levels with slightly higher cross sections. The total fast neutron cross section, combining all other types of cross sections, was reported in [7] as between 500 and 800 fm$^2$ for even higher neutron energies.

The large capture cross section for thermal neutrons of hafnium along with the very small total capture cross section for fast neutrons makes hafnium capture thermal neutrons while letting fast neutrons pass through it. The low cross sectional area of all the combined types or total cross section allows most fast neutrons to pass almost unchanged from their initial energy level. Hafnium has been considered in [8] for use as a fuel shielding in fast neutron reactors to protect the fuel from the occasional thermal neutron. The choice in [4] to use hafnium as a shield will reduce the thermal neutron flux to the specimen being shielded. The hafnium shield will also allow higher energy neutrons, which have not been scattered by the hafnium, damage the specimen representing actual conditions in a fast nuclear reactor environment.

1.4 Aluminum

Aluminum is a very common material making it a cheap material because of availability. Aluminum also has a high thermal conductivity moving heat energy very well. Using the same source, [5], as for hafnium, the thermal capture cross section for aluminum was roughly $22 \pm 5\% \text{ fm}^2 \ (0.22 \pm 5\% \text{ b})$. The fast neutron capture cross section from [9] was between the ranges of about 0.1 to 2.0 fm$^2$. The fast neutron total cross section at high energies in [7] is about 100 to 300 fm$^2$. The absorption cross section for aluminum for fast neutrons makes up
a small portion of the total cross section. Scattering is the main form of interaction between aluminum and fast neutrons and is very limited due to the small cross section.

With aluminum in the shield, any heat generated will be removed and transferred to the coolant quickly due to the high thermal conductivity. This is important since new fuel types can and will be tested using the screening shield. Fuel testing generates more heat than regular material testing due to fission. All heat, however, needs to be removed from the specimens and the screening shield. The shield will come into direct contact with the reactor coolant to maximize convection heat transfer from the shield. The shield cannot fail and allow coolant to directly contact an ATR material test. Another benefit of aluminum is there is only one isotope in natural aluminum. This means the behavior of neutrons in pure aluminum is the same anywhere in the material since only one isotope interacts with the neutrons before the aluminum is damaged by the neutrons. This is not the case in hafnium as seen in [6] with different isotopes of hafnium having different cross sections. The aluminum in the shield will not affect the neutron flux greatly since it neither absorbs or collides much with neutrons. This is very important since a short time in a high flux can quickly simulate a long time period in a low flux environment. So the operating life span of a material in a reactor, which can be over 40 years, can be simulated in just months to years.

1.5 A New Design

The Utah State University (USU) shielding composite material, Al₃Hf-Al, specimens are placed within a test capsule constructed from Aluminum 6061 alloy to be exposed to the thermal neutron environment inside the ATR. The capsule design contains a test cap section which allows reactor coolant, water for the ATR, to directly contact the specimens. Direct contact is necessary to conduct the test of the corrosion resistance of the shielding material. Even though hafnium and aluminum are corrosion resistant, it is unknown how the reactor environment and a composite from the two will affect the corrosion resistance of the new material for shielding throughout the life of a specimen shield in the reactor.

The capsules are designed to stack end on end allowing for many to fit within one
experiment basket. This basket is lowered down tubes into position for exposure to radiation from the reactor. The new test cap section design, which exposes the specimens to coolant for corrosion testing, has never been used before. The thermal and fluid behavior in this test cap with coolant must be known to verify a proper corrosion test before placing the experiment into the ATR. The test cap sections were tested by Idaho State University (ISU) to determine the pressure drop associated with the design. The pumping requirements for the test cap and the flow of coolant over the specimens could then be verified from the fluid test.

The test cap was designed to have a lower pressure drop than a design where a solid rod was used instead of the test cap section. The solid rod would not test corrosion and is used to house non-corrosion specimens during testing inside the capsule. The fluid experiment at ISU tested both the test cap and the solid rod to compare pressure drops. The design of the test cap used parallel flow paths for the coolant to achieve a lower pressure drop than a single flow path found when using a solid rod. Usually parallel flow paths reduce the pressure drop, but the fluid experiment conducted by ISU showed the opposite of what intuition thought would happen. The solid rod had a lower pressure drop than the test cap section. Further study into this counterintuitive flow of coolant was needed to explain why it was not behaving as expected for a parallel flow design.

The problem with the fluid experiment results was they went against intuition and the current understanding of parallel flow. The test cap section was designed with parallel flow in mind. Either the test cap section failed to be a parallel channel flow or the ISU fluid experiment was flawed. The test cap section would fail if flow failed to enter the inside and contact the specimens. This would eliminate the parallel channel and would prevent a proper corrosion test. The whole purpose of the test cap section was to allow for direct contact of flowing fluid with the specimens for corrosion testing while under radiation bombardment.

A review of the design and ISU fluid results will be given below. The reasoning behind using a parallel flow design will be proven. The disagreement between what was expected for the pressure drop and the actual experimental results was the main cause of concern of the
test cap section not preforming its designed role as a corrosion test method. A simulation of the flow conditions will be used to explain the pressure drop anomaly and to show the validity of the test cap section as a corrosion test specimen holder.

1.6 Literature Review

The study of pipe flow has been a major part of fluid dynamics. However, no previous work was specifically found about abnormal pressure drops in a parallel flow design. The parallel channel flow characteristics are well known. The literature referenced addressed the proper method of simulation and different types of pressure losses.

The theory behind parallel channel flow was taken from [10]. The test cap design features four channels which separate and then rejoin. The only difference between a classic parallel channel flow described in [10] and the test cap design is the separated channels from the four gap channels are allowed to mix with each other inside the test cap section where the specimens are located. This difference required the ISU fluid experiment to see if the fluid behaved as predicted by parallel flow theory.

According to the advice given in [11], polyhedral mesh elements should be used on complex industrial components. The complex shapes studied and simulated showed the value of using polyhedral elements when the geometry could not be easily meshed using hexahedral elements. The industrial components used as case studies showed proper simulation technique of setting up the mesh and visualizing the data. The use of importing a solid model as the starting geometry was suggested here as well.

Even though [11] suggested the use of polyhedral elements, [12] showed the benefit of polyhedral elements when compared to other types of mesh elements. The accuracy of tetrahedral, polyhedral, and hexahedral mesh elements was compared and described. It was shown that the easiest to mesh was tetrahedral elements, but they provided the worse accuracy. The next easiest to mesh was polyhedral elements, and they had an accuracy slightly less than hexahedral elements. Hexahedral elements were shown to be the hardest to mesh as they required the most user control, but they offered the best accuracy.

The ability of tetrahedral elements to model complex geometries very well was shown
in [13]. The tetrahedral elements could handle concave, convex, and intersections as long as the element size was small enough to resolve small geometries. The great thing about tetrahedral elements being able to represent complex shapes was that polyhedral elements are generated from tetrahedral meshes. This allowed for a good representation of the test cap section with a better accuracy.

The method, described in [14], simulates flow through orifices which the test cap section openings resemble. The similarity in geometry was limited just to the separation area. Flow through an orifice produced a pressure drop in the study. Pressure drop from orifice flow was a possible contributing source of the abnormal pressure drop.

The flow of fluid in a gap channel and the simulation of such was addressed in [15]. A long capsule was moved down a pipe. The capsule diameter was less than the inner diameter of the pipe creating a gap for fluid to flow by as the capsule moved down the pipe. This small gap geometry was very similar to the gap geometry of the channels in the simulation.

The pressure loss from mixing with no moving parts was studied in [16]. According to [16], it was found that with a relatively little sacrifice of cross sectional area in a pipe and no moving parts, mixing could produce a high pressure drop. Mixing inside the test cap section was expected as a result of the complex geometries.

Pressure loss for sudden contractions was studied in [17]. This study used both a non-Newtonian fluid and a Newtonian fluid. The Newtonian fluid results applied to the test cap section as the working fluid was water. The study found pressure loss through sudden contractions, and this was supported in [18]. The reference text, [18], not only presented fluid theory supporting a pressure loss through sudden contractions and expansions, but also in gradual contractions and expansions resembling nozzle designs.

1.7 Objectives

Using the information from literature, the simulation of the new test cap design was conducted. The objectives for the simulation were to:
• Verify flow through the test cap section which provided direct contact of the coolant with the specimen for corrosion resistance testing.

• Provide support for or counter evidence against the results of the ISU fluid experiment. The pattern would agree even if the magnitudes of the pressure drops do not. Opposite patterns would show the ISU fluid experiment was flawed.

• Analyze the fluid flow for possible contributing factors to the pressure drop anomaly.

Simulation was a valuable tool to complete these objectives. The freedom of exploring the flow using simulation was constantly used to see the complex flow in 3D. Planes cutting the simulation geometry were used to simplify the results since paper is a 2D medium. Caution was used to determine if small vectors were instead large cross plane flow indicators. The majority of flow was mostly in plane. The fluid experiment did not have the freedom to explore flow leaving the objectives listed to the simulation.
Chapter 2

Fluid Experiment

The original fluid experiment by ISU was conducted to show the new design did behave like a parallel flow system as was intended by the designers. The flow is important to the cooling of the material test in the reactor and a proper corrosion test of the hafnium aluminide composite shielding material. Failure to cool the test could result in the melting of the entire assembly or a failed corrosion test wasting an entire test cycle in the reactor. The experiment could show, based on the pressure drop, if the coolant was indeed behaving as expected before the material test was placed into the reactor.

When the results from the fluid experiment were the opposite of what was expected from the parallel flow channel, concern of the cooling capacity of the test cap and the coolant flow was questioned. However, the worst case scenario is having no flow of coolant. No flow of coolant means only conduction cooling instead of convection and conduction cooling working together. It was found by a thermal analysis conducted by Idaho National Laboratory (INL) of the design that the worst case of no coolant flow could still cool the test through conduction only since this was not a fuel material test. This left only the flow anomaly to be explained and the proof of coolant flow through the test cap to properly test the corrosion of the specimen.

2.1 Physical Appearance

The new design consists of a three parts: a basket, a test rod with non-corrosion test specimens inside, and a test cap holding the corrosion specimens. The test cap can be attached to the test rod. This modular design allows for modifications and flexibility. Together, the test rod and test cap fit inside the basket and the whole assembly is a test capsule containing many different specimens for placement in the reactor. The assembly
Fig. 2.1: Isometric view of one end of the test capsule cage.

can include the test cap section or not because of the modular design. The gap between the test rod and basket is where coolant flows in order to cool the entire test capsule. The test cap allows this gap coolant to flow into direct contact with the material specimens held in holders inside the test cap. This direct interaction with coolant does not happen in the test rods. All of the assembly is subjected to the nuclear reactor environment. The test caps are designed to operate in pairs. One test cap lets the coolant flow into where the specimens are being held and the other lets the coolant flow out to rejoin the gap coolant. Gap fluid also flows outside the test cap since there is room there as well. These two flow paths create the parallel flow the designers hoped would reduce the pressure drop across the test cap pair. Test capsules are usually placed end to end to achieve this flow condition. The fluid experiment and later simulation examined only one such pair of test capsules, though many could be used in a full test capsule when lowered into the ATR.

The basket, shown in figure 2.1, looks like a simple pipe with four bumps. These bumps hold the test rods and test caps centered when placed inside. They also provide the gap for
the coolant fluid to flow through. The test rods from the outside look nothing more than just solid rods. Inside, not exposed to the coolant, are specimens, which were placed before sealing the test rod. Since coolant is not exposed to any of these specimens, they are not important to simulating the fluid flow. The test caps fit on the end of these rods as shown in figure 2.2. The test caps are the opposing sections in the middle of figure 2.2 with grooved openings into the center section of the test cap. This assembly fits inside the basket in figure 2.1, and fluid flows around the outside of the test rods and test caps. Cooling fluid also flows inside the test caps via the grooved openings and contacts the specimens for the corrosion test. The placement of the specimens in the holders without showing the test caps is shown in figure 2.3. The specimens are the thin flat discs held by the three prong holders. Each test cap can contain up to three specimens. The asymmetric placement of the specimens requires a full model simulation without any mirror boundary conditions. The complicated geometries and obstructions almost guarantee a turbulent flow of coolant inside the test caps.
The design was made to use parallel flow produced by coolant flowing inside the basket in the gap between the test rods and the outside of the test caps and through the inside of the test caps where the specimens are located. The fluid inlets and outlets can be seen in both figures 2.2 and 2.3. The cut out ramps in the test rods with the open arch of the test cap allow the fluid to flow easily into and out of the corrosion testing region inside the test cap.

2.2 Design

The fluid experiment measured the pressure drop between two pressure taps in the basket. The pressure taps were located 0.0254m (0.5 in) from the end of each test cap. This placed the pressure taps in symmetric locations when the two test caps are placed end to end. These two pressure taps were then attached to a pressure transducer. A flow meter just upstream of the test section containing the assembly gave the flow provided by a
In order for a simulation to accurately represent an experiment, the physical conditions present must be known. The working fluid in the experiment was water at room temperature. The ATR reactor coolant is water. The properties of water were assumed to be constant during the experiment. Temperature change and physical property change because of temperature in the water was assumed negligible for this flow experiment. There was no phase change of the water in the fluid experiment, and there should not be any phase change of the coolant water in the ATR test tubes.

The experiment has three major parts. The first is the basket. The basket has coolant flowing inside it. The basket is basically a pipe except for the four bumps running down the length of the pipe. The bumps support the test rods of specimen or other solid rods of the same diameter. This also allows coolant to flow down the outside surface of the capsule or solid rod as shown in figure 2.5, where the fluid flow through the cross section is pointed out by the label. The flow area cross section is $75.025\,\text{mm}^2$. Figure 2.5 has the basket containing either the test rod or solid rod placed in the center position. The assembly has the majority
of the flow blocked with either rod type being used. The fluid experiment would switch the assembly with the test caps with the assembly with a solid rod replacing the test caps. Both look the same from the end shown in figure 2.5.

2.3 Parallel Flow Pressure Drop

The assembly was expected and designed to behave as a parallel channel flow when compared to a single channel flow. The behavior desired can easily be seen when doing a pipe flow analysis using the modified Bernoulli equation on a parallel pipe system made from two pipes as shown in figure 2.6 as done in [10]. The modified Bernoulli equation from
point \( A \) to point \( B \) along pipe 1 is

\[
\frac{P_A}{\rho g} + \frac{V_A^2}{2g} + z_A = \frac{P_B}{\rho g} + \frac{V_B^2}{2g} + z_B + \frac{f_1 L_1 V_1^2}{D_1 2g} + \sum K_1 V_1^2, \quad (2.1)
\]

where subscripts denote location of the value, \( P \) is the pressure, \( \rho \) is the fluid’s density, \( g \) is gravity, \( V \) is the fluid’s average velocity, \( z \) is the vertical height from some reference datum, \( f \) is the friction factor, \( L \) is the pipe length, \( D \) is the pipe diameter, and \( \sum K \) is the sum of the minor losses. Pipe 2 has a similar equation.

A few assumptions can simplify equation 2.1 to make this hypothetical system easier to follow while still showing the behavior of parallel flow against single channel flow. The first assumption is the same inlet and outlet diameters at \( A \) and \( B \), which means \( V_A = V_B \). The second assumption is the system does not change elevation from \( A \) to \( B \), which means \( z_A = z_B \). The third assumption is the minor losses are negligible, which means \( \sum K = 0 \). Equation 2.2 relates velocity to flow rate as

\[
V = \frac{Q}{A}, \quad (2.2)
\]

where \( Q \) is the flow rate and \( A \) is the cross sectional area of the pipe where fluid would flow.

Using the assumptions made, using equation 2.2, and simplifying the result makes equation 2.1 give the pressure drop, \( \Delta P \) or \( P_A - P_B \), across pipe 1 as

\[
\Delta P_1 = \frac{8 \rho L_1}{\pi^2 D_1^5} f_1 Q_1^2, \quad (2.3)
\]

where \( \pi \) is just the constant and comes from relating the area of a circle to the diameter. The pressure drop across pipe 2 is similar to equation 2.3. An iterative approach must be taken to solve both pipe 1 and pipe 2 equations using the knowledge that \( Q_{inlet} = Q_1 + Q_2 \) shown in figure 2.6 and \( \Delta P_1 = \Delta P_2 \).

The single pipe looks much the same as the system in figure 2.6, except pipe 2 is not there, which means \( Q_{inlet} = Q_1 \) in a single pipe flow case. Using the same assumptions and
same approach, the pressure drop of a single channel flow is

\[ \Delta P_1 = \frac{8 \rho L_1}{\pi^2 D_1^5} f_1 Q_{inlet}^2, \]  

(2.4)

where the only difference from the parallel pipe flow is the flow rate \( Q \), being \( Q_{inlet} > Q_1 \). With the friction factor, \( f \), dependent on flow rate, a hypothetical numerical simulation was performed. \( Q_{inlet} \) was varied and the pressure drop was recorded for both parallel and single flow pipe systems. Figure 2.7 clearly shows the pressure drop for the single channel is greater than for parallel channel flow and the two lines do not cross.

2.4 Counterintuitive Result

The actual fluid experiment did not produce results similar to figure 2.7. The experimental procedures and results can be found in [19], which is the full experimental report from ISU. Here will only be a brief summary of the results. Figure 2.8 displays the results obtained when testing both the test cap section and the solid rod. The magnitude of the pressure drop would have been important except for the relative position of the two lines.
Fig. 2.8: Results of pressure drop for the solid rod and test cap section test.

The most important result from the experiment was the test cap section’s pressure difference was higher than the solid rod’s pressure difference. The trends of both sets of data are as expected. This test gave a result without an explanation of what was happening in the single channel (solid rod) and parallel channel (test cap section) flows.

Those who conducted the experiment were at a loss of how to explain the results. The experimental setup was not transparent. The flow could not be seen inside the test cap section. The result was just the opposite of what was expected producing suspicion of proper flow during the experiment. The parallel channel flow should have a lower pressure drop than single channel flow. This can be proved with Bernoulli’s equation. The design had failed to behave as expected. Proof was needed to show the fluid was flowing through the test cap section in order to properly test corrosion. The resources at USU will be used to run a Computational Fluid Dynamics (CFD) simulation of the fluid experiment.
Chapter 3

Simulation

Because of the need to actually see the flow, a simulation is perfect to explain the results of the experiment and visualize the flow. Modern CFD software can also allow users to see through walls, track streamlines, compute various fluid properties, show vector and pressure fields of the flow, and explore the effects on the flow of geometric changes in the structure. Simulation is also usually cheaper and easier to change than a prototype for testing. However, simulation could have errors in the solution making it not match the physical world.

3.1 Governing Equations

The well know Naiver-Stokes equations define the physics of the real world in the language of mathematics. The flow simulated was a constant-property and incompressible flow. The Navier-Stokes equations, provided by [20], for this simplified case are:

- Continuity equation:
  \[
  \frac{\partial u_i}{\partial x_i} = 0 ,
  \]

- Momentum equation:
  \[
  \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial t_{ij}}{\partial x_j} , 
  \]

where the subscripts denote Einstein notation. \( u_i \) is the velocity vector, \( x_i \) is the position vector, \( t \) is time, and \( t_{ij} \) is the viscous stress tensor. This tensor is given by \( t_{ij} = 2\mu s_{ij} \), where \( \mu \) is the viscosity and \( s_{ij} \) is the strain rate tensor defined as

\[
  s_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) .
  \]
Reynolds time averaging, $\phi(x,t) = \bar{\phi}(x) + \phi'(x,t)$, is used to statistically model the turbulent motion of the fluid with $\phi$ representing the variable in question, which would be the velocity with lowercase $u$ representing the instantaneous velocity. $\bar{\phi}$ is the average value with a capital $U$ denoting the mean velocity. $\phi'$ denotes the turbulent fluctuations to the steady mean flow and represented by $u'$.

By applying time averaging to equations 3.1 and 3.2, the Reynolds-averaged Navier-Stokes (RANS) equations are given as

$$\frac{\partial U_i}{\partial x_i} = 0, \quad (3.4)$$

$$\rho \frac{\partial U_i}{\partial t} + \rho U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left( 2\mu S_{ji} - \rho u'_j u'_i \right), \quad (3.5)$$

with capital letters denoting the mean value. It should also be noted that the viscous stress tensor is now represented by $t_{ij} = 2\mu S_{ij} - \rho u'_j u'_j$. The last term in the viscous stress tensor is the Reynolds stress tensor given as

$$\tau_{ij} = -\bar{u'_i u'_j}. \quad (3.6)$$

The reference text, [20], showed that when deriving the transport equation for the Reynolds stress tensor, 22 new unknowns are introduced. This process can then be repeated for the new unknowns which also introduce even more new unknowns. To avoid this, the Boussinesq approximation of turbulent stresses being linked to average flow variables replaces equation 3.6 as

$$\tau_{ij} = 2\nu_T S_{ij} - \frac{2}{3}k\delta_{ij}, \quad (3.7)$$

with $\delta_{ij}$ being the Kronecker delta. Different turbulent models handle equation 3.7 differently in defining and transporting $\nu_T$ and $k$. 
The turbulence model chosen was the realizable k-\(\epsilon\) turbulent model outlined in [21]. The kinetic energy of the turbulent fluctuations, \(k\), in the flow is defined as

\[
k = \frac{1}{2} \bar{u}_i u'_i .
\] (3.8)

The dissipation per unit mass, \(\epsilon\), is defined as

\[
\epsilon = \nu \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_k}{\partial x_i},
\]

where \(\nu\) is the kinematic viscosity. The k-\(\epsilon\) turbulent model is a two-equation model, meaning it uses two transport equations. The first equation is the turbulent energy equation given by

\[
\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = \tau_{ij} \frac{\partial U_i}{\partial x_j} - \epsilon + \frac{\partial}{\partial x_j} \left[ \nu + \frac{\nu_T}{\sigma_k} \right] \frac{\partial k}{\partial x_j},
\] (3.9)

where the kinematic eddy viscosity is \(\nu_T = C_\mu k^2/\epsilon\). \(C_\mu\) and \(\sigma_k\) are closure coefficients. The second equation is the turbulent dissipation given by

\[
\frac{\partial \epsilon}{\partial t} + U_j \frac{\partial \epsilon}{\partial x_j} = C_{\epsilon 1} \frac{\epsilon}{k} \tau_{ij} \frac{\partial U_i}{\partial x_j} - C_{\epsilon 2} \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left[ \nu + \frac{\nu_T}{\sigma_\epsilon} \right] \frac{\partial \epsilon}{\partial x_j},
\] (3.10)

where \(C_{\epsilon 1}\), \(C_{\epsilon 2}\), and \(\sigma_\epsilon\) are closure coefficients. Closure coefficients are usually constants found to fit the equation to empirical data from varying sources.

The realizable k-\(\epsilon\) turbulent model replaces \(C_{\epsilon 1}\) and \(C_\mu\) as being constant closure coefficient values to being computed values during the simulation as seen in [21]. Equation 3.10 becomes

\[
\frac{\partial \epsilon}{\partial t} + U_j \frac{\partial \epsilon}{\partial x_j} = C_{\epsilon 1} S \epsilon - C_{\epsilon 2} \frac{\epsilon^2}{k} + \sqrt{\nu \epsilon} \frac{\partial \epsilon}{\partial x_j} \left[ \nu + \frac{\nu_T}{\sigma_\epsilon} \right] \frac{\partial \epsilon}{\partial x_j},
\] (3.11)

where \(S = \sqrt{2 \tau_{ij} S_{ij}}\). The rest of the closure coefficients are \(C_{\epsilon 2} = 1.9\), \(\sigma_k = 1.0\), and \(\sigma_\epsilon = 1.2\).

### 3.2 Finite Volume Method

The integration of a transport equation about a control volume is the finite volume
method. If the flow in question is divided up into a grid with each element representing a control volume, then the finite volume method would produce a solution field of values at each volume node for the interested variable. The general form of a transport equation for the general variable \( \phi \) is found in [22] of the form

\[
\frac{\partial (\rho \phi)}{\partial t} + \nabla \cdot (\rho \phi \mathbf{u}) = \nabla \cdot (\Gamma \nabla \phi) + S_{\phi},
\]

(3.12)

where \( \mathbf{u} \) is the velocity vector, \( \Gamma \) is the diffusion coefficient for \( \phi \), and \( S_{\phi} \) is the source term. When equation 3.12 is integrated about a control volume, the Gauss’s divergence theorem is applied, and the transient term is dropped because the simulation is steady state, the result becomes

\[
\int_{A} \mathbf{n} \cdot (\rho \mathbf{u} \phi) \, dA = \int_{A} \mathbf{n} \cdot (\Gamma \nabla \phi) \, dA + \int_{CV} S_{\phi} \, dV,
\]

(3.13)

where \( \mathbf{n} \) is the normal vector to the surface \( A \). \( CV \) is the control volume integral of the volume \( V \). The first term in equation 3.13 is named the convective term. This term tracks the movement of \( \phi \) through the surface of the control volume by convection. The second term is the diffusion term tracking the amount of \( \phi \) moved through the surface by diffusion. The third and last term is the source term providing for the amount of \( \phi \) created or removed in the control volume. The source term discretized at the mesh element volume’s center becomes \((S_{\phi}V)_{0}\). The diffusion term discretized at the face \( f \) becomes \( D_{f} = \Gamma_{f} \nabla \phi_{f} \cdot \mathbf{a} \), where \( \mathbf{a} \) represents the area vector. The convective term discretized at the face \( f \) of the mesh element as \( \dot{m}_{f} \phi_{f} \).

### 3.3 Process

Commercial CFD software was used to conduct the simulation. The commercial software has already been validated and verified to solve the governing equations and to properly use the simulation models. STAR-CCM+ from CD-adapco version 6.04.014 of STAR-CCM+ was used on a computational cluster to provide parallel computation to reduce simulation time. Cluster computation is a common practice for CFD simulation and has allowed for
larger, more complicated simulations to be run.

The start of any CFD simulation is the mesh or grid of nodes which represent the volume the fluid will occupy. The start of the mesh began with deciding whether the type of flow was either internal or external. This simulation was an internal flow inside the basket. The actual mesh started from the solid model of the assembly saved in an IGES file format. The solid model was used during fabrication of the actual tested part during the ISU fluid experiment. This solid model was imported into STAR-CCM+ as a surface mesh with each part of the model being a different region. The sewing tolerance was 0.0001 m.

Certain part regions were either deleted or merged together depending on the needs of the simulation. For example, the solid rod simulation of a solid rod inside the cage did not need the specimen regions or test cap regions. Merging of neighboring regions also made boundaries continuous even when spanning different imported parts. This was important as the wall boundary spanned multiple imported regions. Visual inspection was made to verify the imported surface retained the necessary detail needed for the simulation to represent the geometry used in the experiment. If a sewing tolerance was too large, then sharp edges would be rounded and certain features could be smoothed or merged into a nearby surface. Visual inspection and the small sewing tolerance insured the mesh looked like the solid model. The solid model was no longer of any use after the mesh was created from it.

For this internal flow simulation, the region needing to be meshed was not the solid regions given by the solid model, but the fluid flow volumes around or between solids. The imported regions inside the basket are the objects the flow would be flowing around. The current mesh of the solid model could be useful for solid simulation, but the interest was in the fluid flow for this simulation. To get the fluid flow regions, the solid regions needed a fine mesh to prevent virtual leaks during simulation when the fluid mesh is found from the solid mesh. The objects and space inside the basket basically needed to be switched so the objects would be empty space. Then the original space would be meshed where the fluid would flow.

STAR-CCM+ uses a surface wrapper to improve the imported surface mesh and to do
leak detection. During leak detection, the ends of the basket region were sealed by forming a mesh cap on each end. These mesh caps would also serve as inlet and outlet boundaries later. The internal volume of the solid model was selected for volume mesh generation instead of the solid model volume. This selection told the software to make a new mesh inside the closed volume created by the solid region surface mesh when creating the new volume mesh. This new volume can be thought of as inverting the solid model. The empty space and mesh of the imported geometry have been switched.

Because of the no-slip condition of fluids next to any wall, a fine mesh with many points was needed near any surface. A fine mesh reduces the error in the final solution. The surface mesh size was changed to produce a finer grid close to any surface. Fine grids next to walls are a common practice in simulations to resolve the boundary layer of fluids. It is very important in turbulent simulations because wall functions are usually used to determine the flow inside the viscous sublayer. The surface wrapper improved the surface mesh which was used as the starting place to generate the volume mesh.

With the internal volume set to be meshed with an improved surface wrapper representation of the model, the imported surface mesh was no longer needed and was deleted along with its unimportant feature curves. Only the internal volume mesh was left for the fluid to flow through during simulation. Boundaries were then created from the remaining surface mesh by grouping split patches. Patches were grouped by hand based on what type of boundary the group would become.

Three types of boundaries were used. The most common type was the wall boundary. Wall boundaries prevent fluid from flowing through them and provide the no-slip condition forming the boundary layers in the fluid. Near wall boundaries, a fine mesh was specified. The mass flow inlet boundary was used to provide the fluid flow conditions at the fluid entrance into the basket. This value would change depending on which flow rate was being simulated. The pressure outlet boundary was used at the exit of the fluid from the basket. The pressure outlet also allowed for recirculation. The pressure outlet let fluid flow out of the simulation or in depending on the needed flow calculated during the simulation. The
outlet could actually be an inlet during simulation if the flow recirculated. Recirculation was not expected for the simulation since the bulk flow was from the inlet and there was only one inlet and one outlet. In an effort not to limit the true solution, recirculation was still possible because of the exit boundary chosen even if recirculation was not expected.

After the boundary surfaces are assigned, the mesh was ready for the final mesh generation depending on what geometry was being simulated, test cap section or solid rod. The full simulation of a test cap section containing the specimen assembly and specimens required no further attention before completing the mesh generation. Only one internal volume existed in this mesh of the full geometry. This volume mesh was computed from the surface mesh. The test cap section mesh was now ready after volume meshing for solution simulation.

The simulation without the test cap sections, the solid rod, required some more preparation to remove the test caps. The entire test cap section had to be replaced by a solid rod. A mesh of a solid rod was used to replace the test cap section before the inverting of the empty space and the solid model. Boolean addition was used to merge the solid rod and the surface wrapped regions together, thereby eliminating the test caps. Four internal flow volumes, the gaps between the basket and rod regions, were then defined as a final step before inverting the solid model and the empty space. Mesh generation for the solid rod geometry proceeded much the same as the test cap section.

3.4 Mesh Generation Properties

To properly simulate the experiment, the grid must match the physics of the experiment and the geometry of the model. The mesh of the model determines how accurate the simulation is and how long the simulation takes to run. Care was taken to spend the time and computation resources at areas in the mesh where important fluid flow was occurring. Too coarse of a mesh would not resolve important fluid flow and would lead to false solutions not faithfully representing real world flow.

As suggested in [11], the polyhedral volume mesh generator was chosen. A polyhedral mesh has many advantages over other mesh types such as tetrahedral or hexahedral volumes. A polyhedral mesh is not limited to a specific number of faces or sides. Polyhedral
elements are more accurate than tetrahedral elements in CFD as proved in [12], but less accurate than hexahedral elements. Hexahedral elements are fairly difficult to geometrically represent a complex geometry without much user specification and time devoted to mesh generation. Tetrahedral elements represent complex shapes well, as shown in [13]. Polyhedral elements are generated from a tetrahedral mesh of an object as stated in [12] and [21]. This relationship let polyhedral meshes represent the complex geometries of the test cap section fairly well. A polyhedral mesh was decided on since multiple mesh geometries were needed for the simulation. Less user input and time devoted to mesh generation allows for more simulation. The polyhedral mesh was easier to implement than a hexahedral mesh, but it was more accurate than the tetrahedral mesh.

To improve the surface mesh generated by the surface wrapper and used by the volume mesh generator, the surface remesher model in STAR-CCM+ was used on the already improved surface mesh from the surface wrapper. The relative minimum size of this mesh was 10% of the base size and the relative target size was 20%. This was done to help account for the turbulent motion of the fluid inside the small spaces of the test cap. An improved surface mesh produced an improved volume mesh for the final mesh.

The base size in STAR-CCM+ is usually set as a characteristic dimension of the model to be simulated. At first, the base size for this simulation was chosen to represent the largest element allowable inside any volume in the mesh. Later, when more accuracy was desired, the base size was reduced to shrink polygonal elements. The final base size was determined by the capabilities of the software and hardware used to run the simulations. This was undesirable but was a reality due to the resources available. Due to the unknown flow field characteristics, the grid was made fine in all areas.

The problem was that too large of a base size did not represent real flow results. Too small of a base size halted the simulation or halted the computation nodes in the cluster. More computational resources were not available and results did provide some understanding of the flow being simulated. The interpretation of the results from the simulation gave reassurance that the base size chosen was indeed small enough to get the needed validity
to real world fluid flow. The patterns of flow matched even if the actual magnitudes of the values did not match. Further refinement would produce better results if future needs dictated it and more computational resources are available.

The finest grid possible from available computation capabilities used a base size of 0.001 m. This fine grid was used in all simulations. The $z$-normal plane of the test cap section mesh is shown in figure 3.1. The mesh shows the areas where the fluid will be so the empty space is the solid model. One material specimen can be seen in this plane as a round empty space. The center area shows the specimen holders, holder screws, and the gap between them. The holder screws are the two opposing vertical empty space areas in the middle of figure 3.1. The two side areas are the gap between the basket and test caps allowing the fluid to flow outside of the test cap. The inlet boundary into the basket is not shown in figure 3.1. The inlet boundary is further up the $y$-axis. The inlet boundary is far enough from the area of interest to allow the flow to fully develop before entering the test cap section. The fluid flowed from positive $y$ to negative $y$. Figure 3.2 shows a very basic drawing of the geometry and flow and does not show the specimens or specimen holders. Figure 3.2 also clearly shows the parallel channel design.

### 3.5 Boundary and Initial Conditions

To match the conditions of the experiment, certain computation models were used throughout the simulation of each geometry. Firstly, the simulation was of the full 3D model. No mirror boundary conditions or symmetric nodes were used. The flow was allowed to be asymmetric. Steady state flow was assumed because the experiment was allowed to achieve steady state before readings were measured. Only the fluid motion was considered so no energy equation was needed. The Segregated Flow model was chosen since the flow was incompressible as suggested in [21]. Water at room temperature was set as the working fluid to match the experiment conditions. The flow was turbulent. Thus, the k-$\epsilon$ turbulent model was chosen as suggested by [14] and [15], whose own simulations share common geometries with this simulation.
Fig. 3.1: Polygonal volume mesh of test cap section shown in the z-normal plane.
Boundary conditions were matched with the needed flow rate for each specific experiment conducted. The mass inlet boundary condition needed a mass flow rate even though the fluid experiment used a volume flow rate. The volume flow rate was easily computed into a mass flow rate by

$$\dot{m} = Q \cdot \rho,$$

where $\dot{m}$ is the mass flow rate, $Q$ is the volume flow rate, and $\rho$ is the density of the fluid. This computed mass flow rate was specified at the inlet boundary for each simulation run. The outflow boundary was specified as a pressure outlet allowing for flow either from or into this boundary. No mass flow rate or volume flow rate was needed for this type of boundary condition.

Both inlet and outlet boundaries were distanced far away from the locations where the pressure taps were located. The distance allowed the flow to fully develop the boundary layer from the inlet before reaching the area of interest, the test cap section and the pressure taps. The outlet boundary was far enough downstream not to produce a false flow condition on the pressure taps.

The pressure tap holes were not modeled in the simulation even though they were present in the fluid experiment. No pressure tap holes accurately represent the conditions present in actual use in the reactor. The pressure was measured in the simulation in the
same location as the pressure taps in the fluid experiment by using two cross-sectional planes. The planes were oriented perpendicular to the axial direction of the basket, which was also the main direction of the flow. Each plane, one upstream and one downstream from the test cap section, reported back the surface average static pressure. These planes did not influence the flow in any way unlike the actual pressure taps in the fluid experiment. The maximum pressure drop between the average static pressures of the two planes was then reported and compared to the experimental pressure drop. Many variables would cause the simulation and experimental pressure drop values to disagree. However, the pattern and relative magnitudes agreed fairly well. The order of magnitudes of the values was well within the believable realm.

3.6 Convergence Criteria

The traditional method of finding the solution to a CFD simulation is to use the residuals of each equation solved. The residual is a measure of the error left in the simulation. The smaller the residual means the smaller the error in the solution of the flow. The continuity equation is a standard residual to monitor because a lower continuity residual means the better the simulation satisfies the law of conservation of mass. The solution was run until the continuity residual was below $5 \times 10^{-4}$. At this time the pressure drop reported by the simulation was checked for variation between iterations.

The change in pressure drop between iterations was the main indicator of a converged solution after the continuity residual. To accurately compare the experiment to the simulation, a steady pressure drop solution in the simulation was used to judge convergence. Since the fluid experiment took a pressure drop reading at steady state, the simulation pressure drop must also be steady and the solution was converged. Convergence was achieved when changes between iterations for pressure drop was below 0.6898 Pa ($1 \times 10^{-4}$ psi). This change was randomly negative or positive showing no noticeable increase or decrease in the value over many iterations. The positive changes must have been about the same average magnitude as the average negative changes to keep the pressure drop at about the same value for many iterations.
Chapter 4
Pressure Drop Result

4.1 Simulation

With the fluid experiment already completed, simulations of each fluid experiment flow rate and geometry were run on the computation cluster. Figure 4.1 shows both the experimental results and the simulation results. Even though the magnitudes of the pressure drop did not agree between experiment and simulation, the patterns did agree. The major agreement was the relative position of the solid rod and the test cap section. Both exhibited the same behavior of producing results contrary to the intuition shown in figure 2.7. However, at low flow rates, the lines do cross and the parallel channel does have a smaller pressure drop as expected by intuition of parallel pipes. However, this was below $0.00019 \text{m}^3/\text{s}$ ($3 \text{gpm}$) and was not tested during the fluid experiment. The exact location of line intersection could not be found as the pressure drop values between the fluid experiment and simulation don’t agree. The simulation gives the line cross at a value that cannot be trusted because it does not agree with the fluid experiment at other values in figure 4.1. At $0.000063 \text{m}^3/\text{s}$ ($1 \text{gpm}$), the simulated results showed the solid rod to have a pressure drop of 869 Pa ($0.126 \text{psi}$) and the test cap section to be 717 Pa ($0.104 \text{psi}$). Extra simulation outside the flow rates used in the fluid experiment did not show any break in the pattern in faster flow rates. Only the slow flow rates agreed with intuition and did break the pattern shown by the fluid experiment of going against intuition.

The grid resolution could vary the final converged solution. Because of the complexity of the geometry of the model being simulated, the amount of memory used to produce a grid converged solution was beyond the resources available. The simulations still showed the pattern agreement of figure 2.8. Figure 4.2 shows the effect grid resolution has on the recorded pressure drop. If a finer grid resolution was used then a higher pressure drop would
Fig. 4.1: Pressure drop of both experimental setup and simulations.

Fig. 4.2: Pressure drop simulated at 0.000694 m³/s varying by base size.
be computed. This is promising behavior since the simulation results were always lower than the fluid experiment results. The change was more evident on the complex test cap section model than on the solid rod model. The test cap section model had a more complex flow which needed a finer grid than the solid rod model. This suggests the magnitude error of the solid rod error was not greatly caused by lack of grid refinement, but by other sources such as an idealized fluid and surface roughness in the simulation.

To quantify the error introduced into the pressure drop, the grid-convergence index (GCI) was used as given in [23]. The factor of safety used was 1.25 as three points were used. GCI uses Richardson extrapolation to approximate the pressure drop the converged simulation appears to be approaching as grid size goes to 0. This value is then used to estimate the error on the finest grid. The actual pressure drop value would be inside this bounding error box if the grid size was allowed to be near zero.

The GCI for the test cap section was 8.17% and for the solid rod was 1.32%. When applying the error box to the simulation, the errors did not cause the pattern to change. Even with the worse error, the test cap section pressure drop line still did not cross the solid rod pressure drop line. The pattern shown in figure 4.1 was not affected by error. The lines for both simulations were separate enough to be outside each line’s error bounding box.

The test cap section was the area where the pressure drop anomaly occurred. Figure 4.3 shows two velocity vector fields and specimen locations in the flow at 0.0005 m³/s (8 gpm) flow rate, which is at a middle range of flow rates simulated.

4.2 Further Simulation

Because the specimens, specimen holders, and screws produced a rather large obstruction to the flow, a hypothesis of the specimen holding assembly creating a blunt body pressure loss was put forward and needed to be tested. To explore this option, another simulation using the test cap section was done without the specimens, specimen holders, and screws inside the test cap section. This simulation required a completely new mesh to be created from the new geometry. The inside of the test cap section became a large empty space allowing fluid from the gap flow to mix before separating and rejoicing the gap fluid.
Fig. 4.3: Velocity vector flow at 0.0005 m$^3$/s for (a) z-normal plane and (b) x-normal plane.

Table 4.1: Pressure drop comparing test cap section with and without the specimen holding assembly and solid rod simulations at 0.0005 m$^3$/s.

<table>
<thead>
<tr>
<th>Simulation Type</th>
<th>Pressure Drop</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test Cap Section with Specimens</td>
<td>23159 Pa</td>
</tr>
<tr>
<td>Test Cap Section without Specimens</td>
<td>20698 Pa</td>
</tr>
<tr>
<td>Solid Rod</td>
<td>15906 Pa</td>
</tr>
</tbody>
</table>

The simulation was run under the same conditions as the full test cap section and solid rod simulations. Table 4.1 shows the three values from each simulation run with the flow rate set at 0.0005 m$^3$/s (8 gpm). The specimen holding assembly was not responsible for the counterintuitive behavior of the flow, but it was responsible for some of the pressure drop. The flow either lost pressure when blocked by the samples or when diverted to an alternate flow path by the samples. The difference between simulations of the test cap section and the solid rod was about 6895 Pa. The difference the specimens holding assembly produced in the pressure drop was about 2068 Pa. About 12% of the pressure drop could be attributed to the flow interaction with the specimens, specimen holders, and screws at 0.0005 m$^3$/s (8 gpm). Figure 4.4 shows the vector flow field without the hindrance of the blunt body effect from the specimens.
Fig. 4.4: Vector flow field at $0.0005 \text{m}^3/\text{s}$ without the specimen holding assembly in the $x$-normal plane.
Chapter 5
Discussion

The simulation was able to assure there was in fact fluid flow through the test cap section which would directly contact the specimens. The simulation showed the design could still conduct corrosion material tests with a higher than thought pressure drop. If a specific flow rate was needed through the test cap section, the simulation could help determine the inlet flow rate to produce the needed coolant pumping requirements. Figure 4.3 clearly shows vectors of flow inside the test cap section.

An explanation of what mechanism was causing the counterintuitive pressure drop would be beneficial to help with a future design of a corrosion test cap section. The short answer supported by both the fluid experiment and simulation was the Navier-Stokes equations are satisfied by the flow producing the given pressure drops. This short answer did not provide the answer to what specific part of the flow model was responsible for the larger than expected pressure drop. Some hypotheses of contributing factors were considered.

The first was that there was a flow blocking jet exiting from the test cap section. A flow blocking jet could explain the pressure drop anomaly by severely limiting flow out of and, subsequently, into the test cap section. However, every simulation produced vector plots without a blocking jet and showed flow through the test cap section. Figure 5.1 clearly shows the fluid intersection was without a strong blocking jet flow from the test cap section. The flow upstream of the intersection by the basket also did not show any signs of being blocked. The presence of the specimen holding assembly inside the test cap section or the lack thereof also did not produce a blocking jet of fluid as can be seen in figure 4.4.

The blunt body pressure drop shown in table 4.1 provided part of the answer but not all. The pressure drop anomaly was produced by the test cap section geometry and not the samples. A divergent and convergent nozzle or gradual expansion and contraction was
Fig. 5.1: Intersection of fluid from inside and outside the test cap section at 0.0005 m$^3$/s.
hypothesized to provide the pressure drop as it was a geometric feature in every simulation. Using [18], the minor loss coefficients were found for gradual expansions and contractions. The solid model exhibited an expansion of fluid flow volume into the test cap section from the outside cooling channels or gap channel. This expansion then interacted with the specimens and lastly converged back to the size of the cooling channel as it exited the test cap section. This hypothesis supported the findings of the pressure drop not being dependent on whether or not specimens were present in the test cap section shown in table 4.1.

The behavior of fluid in nozzles has already been studied. For incompressible flow, [18] states for a diverging nozzle the velocity will decrease as the pressure increases. When the flow velocity was decreased in the larger cross section downstream of the diverging nozzle, the dynamic pressure from upstream had been converted to static pressure. The opposite is true for a converging nozzle. The velocity increased as the pressure dropped as static pressure was converted into dynamic pressure.

The design of the test cap section entrance and exit models a divergent and convergent nozzle as show by the pressure in figure 5.2 and the velocities in figure 5.3. Even the fluid entering the chamber in the negative x-axis which came in direct contact with a specimen still showed the same behavior as the fluid entering from the positive side. The specimens were rather thin and allowed for entering fluid to easily flow around them out of the plane shown in figure 5.3. The lack of a specimen did produce a much stronger flow on the positive side.

Close inspection of the vector flow fields and pressure fields showed an interesting characteristic occurring in the outer original flow area. Figure 5.4 shows the entrance region velocity field, while figure 5.1 shows the exit region close up. The flow in the original outside channel, the gap flow, first slowed down as part of the flow entered the test cap section. Then the velocity increased as the channel was separated from the test cap section. The velocity again slowed when the test cap section exit contacted the original channel.

The separating and combining of the gap fluid with the test cap section fluid was another hypothesis which could be producing a pressure difference. It was presented that
Fig. 5.2: Pressure field of test cap section at 0.0005 m³/s.
Fig. 5.3: Velocity vectors of test cap section in the z-normal plane at 0.0005 m$^3$/s.
Fig. 5.4: Entrance into test cap section velocity field at $0.0005 \text{m}^3/\text{s}$. 
each could contribute to part of the pressure drop which would eventually produce the higher pressure drop than was expected. Complicated geometries in the simulation produced many flow patterns producing pressure loss which cannot be generalized into simple geometries understood by fluid analysis.

The mixing of the fluid inside the test cap section would provide a part of the pressure drop. The chaotic flow of mixing inside the test cap section was present in all simulations conducted except the solid rod geometry simulations. There was no mixing of the gap fluid in the solid rod simulation since each of the four channels was separated by the bumps on the basket. Pressure loss from mixing fluid could happen just from the geometric design of the object. Mixing can be promoted with little change in the cross sectional area of the flow as seen in [16], but mixing can still provide a pressure drop as long as the fluid flow is chaotic enough.

The flow inside the test cap section was highly chaotic. The pressure loss from this chaotic mixing of the fluid from each of the four outer gap channels contributed to the pressure result in each simulation. Both planes in figure 4.3 showed chaotic flow inside the test capsule when the specimens are present. The flow had a chaotic feel to the field with swirls, splits, and flow into and out of the planes shown.

Compared to the inlet and outlet of the fluid into the test cap section, the cross section of the inside area was greater than the entrance and exit cross section area. This sudden expansion and contraction was after and before the entrance and exits, respectively, into the test cap section and was present in all geometries except the solid rod mesh. Pressure loss due to sudden expansion or contraction of the flow cross sectional area is a common occurrence in pipe flow. Loss coefficients for use in the Bernoulli equation for sudden contractions were studied in [17] for multiple Reynolds numbers. This sudden expansion and contraction was seen by the fluid right before entering or leaving the chamber inside the test cap section from the entrance or exit channels. The channels entrances and exits might have been nozzle-like in design and provided a gradual expansion or contraction, but this ended before the cross sectional area matched the specimen chamber cross sectional area inside the test cap section.
Figures 2.2 and 2.3 can be used to see the size of the relative entrance and exit regions to the volume of the inner chamber of where the specimens are being held.

The last observation of geometry affected flow was only produced when looking at the slower flow rates and comparing them with the higher flow rates. This was extremely important because the pattern was broken between slow and high flow rates. The slow flow rates followed the intuition of figure 2.7 while the fast flow rates used in the fluid experiment produced the opposite effect and gave a pressure anomaly in the designed parallel channel flow. Figures 5.5 and 5.6 show the area where the gap fluid is forced to separate at 0.0005 m$^3$/s ($8$ gpm) and 0.000063 m$^3$/s ($1$ gpm).

Both figures 5.5 and 5.6 have a large white area in the center. This is the outside of the test cap section and separates the gap fluid from the fluid contacting the corrosion specimen, which a part of the specimen can be seen. Figure 5.5 shows the major stream of fluid being forced to the far side against the wall of the basket. Figure 5.6 shows a slight movement of the fluid to the inner wall of the basket, but the fluid is not forced as harshly. The velocity profile in the gap section was more symmetric and spread out in the slower flow rates. The high flow rates exhibited a greater and greater push as speed increased creating more high speed flow towards the wall. This forced concentration of high speed flow near to the wall created a higher pressure drop. The geometry causing such a behavior is present in the simulations where samples were removed causing a pressure drop. This behavior would almost be considered a flow blocking jet, but the jet was not coming from another fluid stream intersecting the gap fluid. The jet like flow was caused by the splitting of the fluid.

Figure 5.7 shows the $0.000063$ m$^3$/s (1 gpm) flow as the fluid rejoins and can be compared to figure 5.1. The concentrated flow at high flow rates, figure 5.1, has not spread back out before intersecting the fluid from the test cap section. The slow flow rate, figure 5.7, did not change as it intersected the rejoining fluid. This further proved there was no jet blocking flow at the rejoining of fluid after the test cap section. This was true at both high and low flow rates simulated.
Fig. 5.5: Zoom of the gap fluid separating at 0.0005 m$^3$/s.
Fig. 5.6: Zoom of the gap fluid separating at $0.000063 \, \text{m}^3/\text{s}$.
Fig. 5.7: Intersection of fluid from inside and outside the test cap section at 0.000063 m³/s.
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Fig. 5.8: Velocity vector flow in test cap section at 0.000063 m³/s.

The concentrated fluid was also seen on the sides which did not have a specimen immediately blocking the path. However, a specimen in the immediate path of the fluid at the entrance into the test cap section, as can be seen in figures 5.5 and 5.6, created a larger force effect on the fluid. This can be seen in both planes shown in figure 4.3 when comparing the side with a specimen to the side without. Even the specimen by the test cap exit in figure 4.3(b) has a small effect, though not as great as the specimen at the entrance into the test cap section. Even at the slower flow rate, the placement of the sample still has an effect on the gap fluid velocity profile, although very small, as can be seen in figure 5.8.

With the gap fluid flow being modified by being forced to one side by a jet-like force, pressure loss not present in the solid rod was added to the normal pressure loss of the rest
of the test cap section and parallel channel flow. This added amount was greater than the pressure savings produced by the parallel channel flow at higher flow rates. At lower flow rates the parallel channel flow did produce more pressure savings and so behaved as intuition predicted. Figure 4.1 showed the higher the flow rate, the less the test cap section behaved as a parallel channel flow. The fluid experiment also showed this as the gap between data widened with increasing flow rates. This behavior of a widening gap with increased flow rate was present in both the fluid experiment and the simulation. As figure 2.7 shows, a parallel channel should not increase as fast as the single channel would. The parallel channel flow helped keep the pressure loss from increasing rapidly as flow rate increased which is more visible in the fluid experiment than the simulation data.

The cause of this interesting fluid flow was found to be caused by the geometry of the entrance region into the test cap section. The entrance and exit have the same geometry, just opposite in facing. Figure 2.2 shows the entrance and exit regions. The specific feature causing the flow to modify the gap fluid was the curved region at the end of the entrance region.

A simple simulation of just the entrance region and exit region allowed for easy changes to the curved feature of the entrance region. The original geometry used a half circle curve at the back of the entrance where the fluid split with part continuing down the gap and part going into the test cap section to contact the specimens. The original curved geometry placed in the simple simulation produced the same disturbance effect on the gap fluid flow as in the full simulation. By changing the half circle to a flat feature or a rectangular ending of the entrance the flow was changed when doing the simple simulation. With the flat back geometry, the gap fluid was hardly affected by the flow splitting. No flow forcing the gap fluid to one side of the gap channel was developed. The flat feature flow behaved the same as flow around a rectangular blunt body.

The curved feature collected the flow and then gathered it to the top of the curved circle. At the very end of the entrance, which was also the top of the curved circle, the flow had to split. Since the flow had been gathered and focused, a large amount of flow
moved into the gap fluid and into the test cap section. The flat feature at the end of the
test cap section did not collect the flow and gather it to one spot. The flow immediately
had to separate and flow into either channel. This spread the flow out so the flow did not
concentrate at one point.
Chapter 6

Summary and Conclusion

As demand for safety, reliability, and efficiency continues to increase for nuclear technology and power, new materials greatly help satisfy these demands. This makes new material testing very important before placement in an actual reactor or structure exposed to nuclear radiation damage. The new specimen shielding material was designed in order to expand the ATR’s capabilities to test high energy neutron environments. The hafnium aluminide composite shielding would allow for fast neutron testing in the BFFL. However, the new design of hafnium aluminide composite itself needed to be tested including corrosion testing. The new capsule design including a corrosion test capability was designed. The new test cap section, allowing corrosion testing, had to be tested for proper fluid flow. The fluid test of the new capsule design using the test cap section produced results counter to the ideas the designers sought.

The designers were trying to use parallel flow to reduce the pressure drop across the test cap section of the testing capsule. The fluid experiment showed the pressure drop was actually more instead of less. This counterintuitive result needed explaining and verification. The flow of the coolant through the test cap section was vital to a corrosion test of the specimen. A simulation of the flow using STAR-CCM+ software was used to show the flow characteristics and the pressure drop anomaly.

The simulation verified the test cap sections did allow the flow of the coolant into direct contact with the specimens for corrosion testing. The vector flow fields of the simulation clearly showed the specimens in contact satisfying the objective for proper corrosion testing flow. There is no stagnate flow inside the test cap section. The flow inside the test cap section even mixed due to chaotic flow. The flow was found to be sufficient for corrosion testing.
The simulation agreed with the results from the fluid experiment proving the fluid experiment was done correctly. The objective was completed by showing supporting simulation results similar to the ISU fluid experiment results. Both results had the pressure drop from the test cap section greater than a solid rod, which was a single channel flow. Only when the flow rate was slow, below the rates used in the fluid experiment, did the simulation show the pressure drop in the test cap section was lower than in the solid rod. The magnitudes of the pressure drops did not agree from fluid experiment to simulation, but the patterns did.

The simulation also gave insight into the contribution the specimen holder assembly had on the pressure drop. However, when removed from the simulation, the pressure drop was still greater than the single channel simulation of the solid rod. This meant blunt body flow interactions were not the primary flow characteristic associated with the abnormal or unexpected pressure drop results.

The geometry of the test cap section had many features which contributed to the pressure drop. A diverging nozzle-like design allowed fluid to enter the test cap section and contact the specimens. A converging nozzle-like design let the fluid exit the test cap section and rejoin the original channel. These factors contributed to the abnormal pressure drop seen in both the physical experiment and virtual simulations. Other contributing factors explored were the sudden expansion and sudden contraction of the test cap section after and before the entrance and exit of the test cap section. The mixing of fluids was thought to also contribute since the flow was highly chaotic inside the test cap section. These disturbances in the flow would provide some contribution to the pressure drop.

The degree of forcing of the gap fluid to the inner wall of the basket as flow rate increased was a noticeable change when comparing velocity vector fields of varying flow rates. The slow flow rates behaved as parallel channels with a lower pressure drops than with the single channel solid rod design. The fast flow rates gave just the opposite. This behavior was only discovered in the simulation as a low enough flow rate was never used in the fluid experiment. This gap fluid modification as flow rate increased produced pressure loss that outweighed the savings produced by the parallel channel design, except at slow flow rates. This gap
flow behavior might be considered a blocking jet flow even though it occurred when the fluid was split. The change of the curved feature in a simpler simulation to a flat feature reduced the gap fluid being forced to the wall. The pressure loss would be reduced if the same flat feature behaved the same way in the full simulation.

With the complex design and the presence of many obstructions and changes to the flow within the test cap section of the test capsules, the total pressure loss with the test cap section was comprised of multiple sources of pressure loss which vary with flow rate. The sum of these sources was able to create a higher pressure drop than a solid rod single channel flow even though the test cap section made use of the parallel channel pipe flow properties.

The current design of the test cap section created the counterintuitive pressure drop. The test cap design would work for corrosion testing only with a higher pressure drop than was desirable unless slow flow rates were used. Future work could be done to minimize the pressure drop by changing the geometry of the test cap section in CFD simulations. Further study into jet blocking flow in the gap fluid could further be understood as it varied by flow rate.
References


