NPACC-X: A Further Evolution of Centrifuge Cascade Analysis

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To my family who supported me along my way and my cats who mostly slept.

Acknowledgments

I would like to thank Howard Hall who first brought me into his group three years ago and Matt Cook who has been a faithful mentor during my time in graduate school. Most of all I would like to thank Dr. David Vermillion who took me on as an undergraduate researcher and introduced me to a new world of nuclear security.

Abstract

The establishment of uranium enrichment facilities is crucial to the development of a peaceful Nuclear Fuel Complex. However, as the industry moved from gaseous diffusion to gas centrifuge technology for increased performance and flexibility, conventional cascade analysis methodologies based on gaseous diffusion were found lacking. The establishment of NPACC under Dr. David Vermillion for his PhD dissertation "Improving Predictive Capabilities of Classical Cascade Theory for Nonproliferation Analysis" sought to remedy the problems posed by the flexible gas centrifuge enrichment technologies. By incorporating newly named "cascade dynamics," he was better able to quantify the capabilities and characteristics of gas centrifuge enrichment plants for nonproliferation analysis. However, this previously built codebase was unable to be obtained by the university and this study seeks to rebuild and recreate those previous results. In this study, the newly developed NPACC-X seeks to recreate the data produced by NPACC in terms of minor isotope separation through a cascade, internal cascade physical parameters, and the analysis of unideal cascade configurations. This study was moderately successful in recreating this previously built cascade modeling tool in that NPACC-X matches the isotopic profiles of the original NPACC with only slight disagreements. However, there still remains differences in the overall isotopic separation factors, hydraulic throughput of the cascade, and isotopic cuts of minor isotopes. Despite these differences, NPACC-X provides The University of Tennessee with previously unobtained cascade modeling capabilities in an open-source format. This serves and the foundation for further work in the area of open-source cascade modeling tools for use in the nonproliferation community in assessing the capabilities, characteristics, and proliferation potential of existing and over-the-horizon Gas Centrifuge Enrichment Plants.

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Chapter 1

Introduction

In order to understand the need for this thesis, it is important to previous work done under David Vermillion for his PhD dissertation "Improving Predictive Capabilities of Classical Cascade Theory for Nonproliferation Analysis." In this dissertation, Dr. Vermillion proposed improvements over traditional classical cascade theory by implementing a new form of cascade analysis incorporating, what he termed, "cascade dynamics." Unfortunately, the original codebase developed in this dissertation has been unavailable for dissemination following his graduation. Therefore, it is important to understand the original background and intent of the dissertation in order to recognize the goals and application of this novel theory. After understanding the motivations behind this aforementioned dissertation, it will be important to explain the need for this study. As stated previously, because the original codebase is not available for the university, it would be beneficial to revisit this dissertation and attempt to recreate the results using only open-source information. This would provide the university with a previously unavailable codebase along with a new form of cascade analysis not openly available to the public.

This study will include a background into the motivations of the original Non-Proliferation Analysis of Centrifuge Cascade (NPACC) code developed by David Vermillion with help from this author. Additionally, this thesis will cover the rebuilding of the lost codebase and introduction of multiple isotope separation, or multi-component, into the original codebase designed for two component separation. Furthermore, this study will

include how to take the existing codebase from Matlab and place it into a more modernized form in Python for ease of use, development, and further improvements. Therefore, it can be thought that this study is a further extension of the work initially started under Dr. David Vermillion. Because this study can be thought of as an extension of previous work, much of the background surrounding the need for gas centrifuge enrichment facilities will be revisited briefly in this introduction. The goal of this author is not to simply copy what was previously stated in Dr. Vermillion's dissertation, but rather give a brief background into how the motivations from his dissertation are the same as the motivations behind this study.

Following the end of the nuclear renaissance in the United States and the Fukishima Daichi nuclear incident, the future role of nuclear power remains uncertain when dealing with a global power demand increase and the increasingly questioned role of fossil fuels due to climate change. The International Atomic Energy Agency (IAEA) estimates that the current global nuclear power capacity of 382.9 gigawatts (GWe) may increase between 1.9-56% in the next 15 years [10]. Despite its uncertainties in developed nations, the IAEA believes that nuclear energy will play a large part in the production of carbon-free, reliable, and economic energy ([11]). In Eisenhower's "Atom's for Peace" speech, he established that all nations have a right to the peaceful use of nuclear energy. However, the Nonproliferation Treaty of 1970 (NPT) dictates that no signatory nation shall develop nuclear weapons technology. Therefore, it is imperative for the international community to foster the development of nuclear power without increasing or aiding in nuclear proliferation.

In order to have nuclear energy, one does not simply build a nuclear reactor, but rather, an entire complex must be built in order to support the continual feed of nuclear fuel to the reactors. This fuel is sourced through the front end of the nuclear fuel cycle (NFC) which includes uranium mines, uranium conversion plants, nuclear fuel fabrication facilities, and uranium enrichment plants. The purpose of this study will be to investigate these uranium enrichment facilities and understand the proliferation challenges that arise when developing peaceful uranium enrichment. The number of these facilities can be expected to increase as the global demand for nuclear power increases; therefore, measures

must be taken to better understand the additional proliferation risks associated with the pursuit of peaceful nuclear power and the expansion of the NFC to other countries.

The most common form of uranium enrichment facility is the Gas Centrifuge Enrichment Plant (GCEP) which is comprised of thousands of gas centrifuges plumbed together so that uranium hexafluoride can be gradually enriched to desired Uranium-235 concentrations necessary for nuclear fuel. This study focuses on the GCEP as other forms of uranium enrichment such as gaseous diffusion have been decommissioned and laser isotope separation processes have been deferred for the time being. These GCEPs are of concern to many lawmakers as their potential proliferation risk is difficult to quantify as how many machines are necessary for a desired production need, how easily can a peaceful GCEP be converted to a proliferation plant, and what safeguards are necessary on these existing plants are all questions that can not be easily quantified.

As laid forth in Dr. Vermillion's introduction to his dissertation, these enrichment facilities pose an unquantifiable risk to the international community. With the established clandestine facilities at Natanx and Fordow, the international community was taken aback by the ability of a foreign actor to covertly develop an undeclared uranium enrichment facility. Although the implementation of the Joint Comprehensive Plan of Action (JCPOA) left size and production rate limitations on these clandestine facilities, it is still unknown as to whether these measures have reduced the proliferation potential of these facilities [14]. This leads to the next problem facing international political actors when dealing with enrichment facilities, the difference between declared and undeclared GCEPs. Declared facilities are enrichment plants that the global community is aware of and can be fitted with proactive safeguard and verification technologies to ensure peaceful use. Undeclared facilities are, by their definition, unknown to the international community, and upon their discovery, can be retrofitted with safeguarding technology. However, both types of facilities are difficult to determine their proliferation risk associated with their operation. Specifically, it is difficult to quantify the risk associated with an undeclared plant and is even more difficult in understanding how to detect and undeclared facility. These undeclared facilities

pose a significant risk to the international community as they have a high proliferation risk and pose a danger to both the neighboring countries and international community at large.

Declared facilities are not entirely risk-free either. Because of the high level of operational versatility associated with these enrichment facilities, declared facilities can still be used to produce weapons-grade uranium (WGU) in a variety of different ways. The manipulation of the physical internals of a cascade, such as the cascade plumbing, can still produce higher-than-declared uranium enrichment without having to change much of the overall look or design of the cascade. Centrifuges themselves offer much in the ways of operational versatility compared to gaseous diffusion and can have their performance altered with the simple manipulation of the cascade, or machine, federate alone. This means that without changing the internal plumbing or operating speeds of gas centrifuges, higher-than-declared uranium enrichments can be achieved by simply manipulating the amount of material being fed to the cascade, and subsequently, the machines. However, because these machines are the definition of a dual-use technology, in that they can be used for both civilian and military purposes, it is important to understand that they pose a significant risk to the international community while still being protected by the NPT as part of a peaceful NFC. It has been established that these peaceful cascades will have enough separation capacity to support peaceful production, but with simple cascade modifications, can be used to support nefarious proliferation production. Therefore, it is imperative that cascade design and operation limitations need to be put into place in order to limit the proliferation potential of these cascades. Additionally, the implementation of both safeguard and verification techniques need to be implemented to ensure that these enrichment facilities are operating in accordance of the operational intent of the given cascade.

In order to uphold the NPT of 1970, technically driven analysis of the GCEP must be performed so that adequate safeguards can be established to ensure peaceful declared enrichment production while also protecting against possible proliferation. This is the fundamental problem that Dr. Vermillion's dissertation attempted to solve. He posited that the cascade is the single indivisible unit of proliferation risk associated with modern

uranium enrichment rather than an individual centrifuge. Therefore, a better understanding of the physical characteristics and improving accuracy associated with the multi-component separation in the cascade will be of great use to the international nonproliferation community. With a better understanding of the physical characteristics of these cascades, better estimations and resticrictions can be passed on the minimum separation capacity of the GCEP to ensure peaceful use while also characterizing clandestine facilities based on the minimum spatial footprint, suspected centrifuge design, perceived end use, and any boundary constraints of the facility (e.g. necessary feed rate, feed type, production rates, amount of tails produced by facility). Although this was thought to be an unattainable idea, Dr. Vermillion's dissertation proved it was possible.

In order to better understand why the improvements in classical cascade theory need to be developed, it is important to understand the currently openly available cascade analysis methodologies available to the nonproliferation analysists. Classical ideal cascade theory was developed by Karl Cohen during the Manhattan Project and was later disseminated in his book "The Theory of Isotope Separation"[3]. This theory was based on gaseous diffusion and served as an analytical solution to the design of a given enrichment facility for a desired production scenario. The methodology derived from classical ideal cascade theory serves as the basis for conventional nonproliferation analysis methods to this day. However, because this theory was developed on gaseous diffusion, ideal cascade theory may not provide enough resolution to accurately predict the design and operation of a conventional GCEP.

Currently, there exists two major methodologies for more accurately estimating GCEPs capabilities and physical characteristics. Firstly, is conventional "ideal black box" analysis in which a theoretical black box can be placed over the entire GCEP and the analyst will look at the material entering and leaving this "black box." This allows the analyst to use the mass flow rate and two component assays associated with the GCEP to make estimations on the capabilities and characteristics of a single cascade using mass and isotopic balance. Secondly, there exists Edward Von Halle's MSTAR technique developed at the K-25 gaseous diffusion plant in Oak Ridge, TN. This methodology seeks to better predict the separation of multi-component isotopic streams as they are passed through and enrichment cascade.

These two analysis methods set the bar as far as openly available cascade analysis tools.

In his PhD dissertation Dr. David Vermillion sought out to develop a more advanced cascade analysis method that would see improve over the aforementioned "ideal black box" and MSTAR [16]. The Non-Proliferation Analysis of Centrifuge Cascades (NPACC), is a program developed to better analyze multi-component isotopic separation as it travels through this enrichment cascade by utilizing numerical calculations of a computer to reach a steady state solution to a given boundary conditions of a cascade. Boundary conditions in this context can include the desired end use, feed stock, tails depletion level, and perceived centrifuge design. It improves over classical ideal cascade theory by the addition of a temporal dimension in cascade performance, accounting for four methods of cascade productivity loss that accompany unideal cascade operations, and a new theoretical method for predicting the separation of multicomponent streams. These principles were referred to as "cascade dynamics." Using first-order machine principles, it uses a simulated annealing optimization routine to let a computer test thousands of different cascade configurations until a most-optimal solution is derived for a given user defined production scenario. This model is designed to be more flexible and provide higher resolution than previously mentioned cascade analysis methods. This methodology has not been discussed in open source literature prior to Dr. Vermillion's dissertation as he provided the seminal description and demonstration of this methodology.

Although a qualitative introduction to cascade dynamics was provided as part of this original dissertation, it is beneficial to restate the conclusions and assumptions provided as part of his study. He posited that by applying cascade dynamics to the analysis of a centrifuge cascade, a newly developed cascade methodology called NPACC would be developed. This new methodology improved the accuracy of traditional centrifuge cascade analysis as well as expanded the state of art uranium cascade analysis. Additionally, it was created specifically to "analyze centrifuge technologies and associated cascade configurations that were proliferated by A.Q. Khan on a turn-key basis"[16]. However, this model was developed in a way that it can be applied to any

future combination of isotope separation technologies and cascade configuration of the future so long as they adhere to the basic first-order principles of separation technology.

NPACC relies on very few input parameters to ensure operational flexibility and easy of use in nonproliferation analysis. Using four user defined parameters, NPACC "numerically estimates the optimum combination of the shape of the hydraulic profile and temporal versatility of a centrifuge cascade necessary to meet the declared or perceived enriched uranium product demand"[16]. It was demonstrated with both natural uranium feedstock and reprocessed uranium feedstock for operational versatility and a greater understanding of the proliferation potential of different forms of uranium feed. Additionally, it is also sensitive to the operational adjustments of acceptable tails U235 which has been shown to follow the global uranium market conditions in order to adhere to economic cascade operations. This assumes that a peaceful GCEP will be operating in an economic fashion.

In the Dr. Vermillion's original dissertation, he covered four different realistic case studies that can cover the a reasonable selection of peaceful demands for enriched uranium. Using the theoretical Rome and Iguacu designs, these results were benchmarked to traditional ideal cascade analysis techniques. This work was done to show the differences between the capabilities of what is currently relied upon and how the introduction of cascade dynamics can be of use to the international nonproliferation analyst community. However, the data produced from his study was not able to be verified or validated due to the fact that this type of information would not be appropriate for an open-academic setting. The results of his study concluded that NPACC, in his form, provided comparable estimates to existing cascade analysis techniques when the assumptions associated with classical cascade theory are met.

As stated previously, the purpose of this thesis will be to recreate wha the original NPACC, in it's final form, methodology concluded. This is because the original program is not currently openly available to academic institutions in its final form. It would therefore be beneficial to recreate this program using only openly available information in order to have a better understanding of multi-component separation in a cascade. However, the

results of this study, similar to Dr. Vermillion's, will be unable to verified or validated due to the lack of empirical data surrounding gas centrifuge enrichment facilities. Due to this author having worked on the previous iterations NPACC under Dr. Vermillion, there is some understanding into the overall development and analysis of the centrifuge cascade. However, this author was not a part of the original multi-component separation implementation into NPACC. It is posited that recreating this code, even if it does not agree with the original, final-iteration version of NPACC's conclusions, it would still be beneficial to the University and other academic institutions in providing a previously unattainable analysis technique. In other words, this author will take the original two component version of NPACC and try to recreate the latest iteration of the cascade code by implementing an open-sourced version of multi-component separation and balancing.

This is not a small feat due to the lack of openly available information on the actual mechanisms by which multi-component streams are separated through enrichment technologies. This study provides relative improvements over the original two component version of NPACC; however, it does not match the conclusions found in the original dissertation by Dr. Vermillion. The purpose of this study will be to describe the current work in updating NPACC form its original two component variation to a similar multi-component variation found in Dr. Vermillion's dissertation. This will cover the existing codebase and its methodology used for analyzing cascades along with the current methodology proposed for balancing multi-component streams. Additionally, this study will cover how to take the original codebase from its origins in Matlab to a more modernized codebase in Python. This modernized codebase would be more flexible and easier to use for future development. It also saves the use of a costly Matlab license which improves this programs availability for future developers.

Finally, a breakdown of the upcoming chapters is warranted. Chapter 2 will cover the uranium feedstock and its enrichment processes along with the openly available centrifuge technologies used for uranium enrichment. Additionally, it will delve deeper into a breakdown of the existing cascade modeling techniques such as ideal black box

and informed ideal cascade theory. Cascade dynamics will be covered in order to gain a better understanding of where the origins of classical ideal cascade theory are derived from, and how the introduction of cascade dynamics can be of use. Additionally, it will include an introduction to the existing codebase developed under David Vermillion for a two-component separation stream. The introduction and implementation of cascade dynamics will be covered in respect to the assumptions of the mathematical procedure and the practical limitations of these techniques as applied to a single gas centrifuge cascade. Here, it is established that black box and informed ideal methodologies are inherently unequipped to answer many questions about declared and undeclared enrichment facilities.

Chapter 3 will be an introduction to the four case studies laid forth in Dr. Vermillion's dissertation and the application of this new version of NPACC to these case studies. Additionally, it will detail the differences and methodologies between the two-component version of NPACC and the current version of NPACC-X developed in this study.

Chapter 4 will be a discussion of the differences between the results of Dr. Vermillion's dissertation and this study. It will include what the perceived reasons are for the differences and what changes could be further implemented to achieve a better estimation of multi-component separation.

Chapter 5 will involve a discussion of how this existing codebase in Matlab can be transformed into Python for further development. Delving into the pros and cons of using Python for this particular model, ways to make the code more flexible, and how its implementation into Python could prove to be a more simplified and easier to understand codebase from a future development standpoint.

Chapter 6 will include the overall conclusions and disclaimers associated with this version of NPACC. Additionally, it will cover the potential benefits of future development.

Chapter 2

Background

Because most reactors in the world rely upon a source of enriched uranium as fuel, this requires some form of natural uranium to be milled, mined, and converted to a form which allows for the enrichment of this material through the front end of a nuclear fuel cycle (NFC). The most common form of this natural uranium comes from simply mining uranium ore out of the earth; however, there are still sizable amounts of uranium contained in the ocean's seawater. Nevertheless, most of the world still relies upon this process of milling, mining, and conversion to UF_6 for use in uranium enrichment cascades. This uranium needs to be enriched because it lacks a sizable enough portion of fissile U^{235} required to sustain a nuclear chain reaction. Because of the lack of fissile U^{235} present in naturally occurring uranium ore, the overall percentage of U^{235} relative to other naturally occurring, non-fissile isotopes such as U^{234} and U^{238} must be increased so that there is a large enough portion of fissile material in the fuel to sustain this chain fission reaction. This is not necessarily the case in every reactor design as reactors such as the pressurized heavy water reactor (PHWR) that can utilize natural uranium as the fuel source. As these reactors pose their own proliferation risk associated with the production of weapons grade plutonium in the core, they will not be of concern in this study, but rather, this study will focus on reactors that require enriched uranium and their subsequent uranium enrichment cascades. Because many reactors require the use of enriched nuclear fuel to sustain peaceful nuclear energy production, there have been many enrichment technologies created to address the problem of uranium isotopic enrichment.

Additionally, there are two other forms of uranium that can be used as feedstock for uranium enrichment cascades and these are reprocessed uranium and excess stockpiled weapons grade uranium. Both of these additional feedstocks can be converted to UF_6 for use in a uranium enrichment cascade; however, reprocessed uranium will only be of concern as weapons grade uranium is usually above the desired enrichments for peaceful power reactors and therefore is simply down-blended with natural uranium to create lowly enriched uranium (LEU) fuel for reactors. This program to convert the highly enriched uranium (HEU) material to LEU fuel was called the Megatons to Megawatts program [1].

Reprocessed uranium will be of great concern in this study because of the presence of minor isotopes such as U^{232}, U^{234}, and U^{236}. This means if an operator were to use reprocessed uranium in an enrichment cascade, these minor isotopes will also be enriched or depleted depending on the cascade shape, configuration, and desired end use. This study will use the reprocessed uranium vector found in Doneddu, Roblin, and Wood's optimization studies for gas centrifuges[5]. The two feedstocks can be found in table 2.1 and 2.2. These minor isotopes are formed from normal irradiation processes found inside a nuclear reactor, and the reprocessed uranium vector used in this study comes from normal light water reactor (LWR) burnups and operating conditions. These reprocessed uranium isotopic levels will vary depending on the level of burnup, reactor design, and operating conditions; however, this study will utilize the reprocessed uranium vector found in "Optimization Studies for Gas Centrifuges" [5].

Table 2.1: Isotopic Characteristics of Natural Uranium [16]

Isotope	Fissile?	Natural wt%	Natural at%
U^{238}	NO	99.284	99.2741
U^{235}	YES	0.711	0.7204
U^{234}	NO	0.005	0.0055

Table 2.2: Isotopic Characteristics of Natural Uranium [5]

Isotope	Fissile?	Natural at%
U^{238}	NO	98.680
U^{235}	YES	0.900
U^{232}	YES	1E-9
U^{233}	YES	0
U^{234}	NO	0.020
U^{236}	NO	0.400

It has been established that uranium enrichment is necessary for a majority of operating reactors, but the level of enrichment necessary and the associated proliferation risks with increasing the fissile content of a uranium feedstock is of concern in this study. As the amount of fissile content increases, so does the proliferation concern due to the increased fissile content resulting in an increased capability of an uncontrolled nuclear chain reaction. Therefore, there should be controls set on the levels of enrichment allowed in a peaceful NFC. The international community uses the IAEA guidelines for the definitions of natural uranium (NU), depleted uranium (DU), highly enriched uranium (HEU), low enriched uranium (LEU), and the detection time necessary for a significant quantity (SQ) of enriched uranium [9]. At or above 20% enriched U^{235} is defined as HEU. This is because around 80% of the separative work, later referred to as separative work units (SWU), is needed to take the material to 20% enriched. And to take the material to weapons grade uranium (WGU) would take the remaining 20% of separative work. Additionally, the depleted tails from an enrichment facility still contains trace amounts of fissile U^{235} and subsequently still requires material accountability and safeguards.

2.1 Enrichment Technology

For the sake of this study, gas centrifuges are the main enrichment technology of concern due to their versatility and availability when planning an uranium enrichment facility. Gaseous diffusion was a prominent enrichment technology prior to the NPT of 1970; however,

following the shutdown of the Paducah Gaseous Diffusion Plant in June 2013 [15], most of the worlds demand for enriched uranium has been met by gas centrifuge technology. This technology accounts for "more than 99% of all commercial and military-dedicated uranium enrichment in the world" [16] [17].

A single gaseous diffusion cell or gas centrifuge does not provide a high level of enrichment in and of themselves. This amount of overall separation between two isotopes is called its "separation factor" and is denoted as α. Therefore, in order to enrich a uranium feed by an appreciable level, these enrichment technologies must be strung together in both series and parallel to ensure adequate enrichment levels along with meeting a desired material throughput. Gaseous diffusion relies on the differences in mass and volume between U^{235} and U^{238} in order to create a pressure differential between the two components against a porous membrane. Under controlled temperature and pressure levels, the U^{235} is preferentially passed to the product stream of a given gaseous diffusion cell. For this process, the separation factor in a single gaseous diffusion cell is very low compared to that of a gas centrifuge. The theoretical maximum separation factor of a gas diffusion cell is around 1.0043 compared to 1.3069 for that of the hypothetical Rome centrifuge [16]. For this reason, Gaseous Diffusion Plants (GDP) are inherently required to be large, continuously fed enrichment facilities that require large amounts of energy and uranium inventory to continually operate. Gaseous diffusion does provide some benefits over gas centrifuge technology in that GDPs can be built in accordance to the assumptions provided in ideal cascade theory. This is because ideal cascade theory was first developed on gaseous diffusion technology and many of the assumptions such as feed rate, cascade stage size, and separation factors will remain constant and can be controlled through normal plant operations. This results in the GDP closely following the designed cascade configuration laid forth by ideal cascade theory. With the large uranium inventory necessary for operation, this results in the GDP having very long equilibrium times on the order of months [16]. This means that in order to justify the construction of a GDP, there needs to be a long-term need for large amounts of enriched uranium material. However, even with these considerations, a GDP is still less economical compared to a Gas Centrifuge Enrichment Plant. For these reasons, most NPT signatories and Nuclear Weapon States (NWS) have moved from gaseous diffusion to gas centrifuge

technology. The only country proposing the development of a GDP to meet its uranium demands is Argentina [17].

2.2 Gas Centrifuge Technology

Gas centrifuge technology relies on the mass differences between U^{235} and U^{238} atoms in a machine rotating at supersonic speeds to create a centrifugal force. Additionally, gas centrifuges will utilize a thermal gradient to increase the effect of buoyant forces on the gas. Simply put, with a vertical temperature gradient, lighter isotopes will rise to the top of the centrifuge and heavier isotopes will sink towards the bottom. This combined with the centrifugal forces acting differently on the different uranium isotopes will result in lighter isotopes being closer to the top centerline of the centrifuge and heavier isotopes will move to the bottom outer wall of the machine. The primary driving mechanism of this separation process is the temperature gradient resulting in taller machines having higher separation factors than their shorter counterparts. In each of these centrifuges, the placement of the machine scoops, or where the material is collected and leaves the machine, is preferentially picked to maximize the collection of light isotopes in the product of the centrifuge and heavy isotopes being passed to the tails of the machine. These thermal and centrifugal gradients result in a two-dimensional separation process which yields higher separation factors than their gaseous diffusion counterpart. As stated previously, gaseous diffusion usually results in separation factors with a maximum around 1.0043 versus a range of separation factors between 1.05 and 1.6 for centrifuge designs [18] [2]. Because of this increased separation factor, gas centrifuge enrichment plants will need fewer enrichment and stripping stages compared to GDPs in order to reach the same level of material enrichment. The reliance on reversible thermodynamic principles result in gas centrifuge technology maintaining operational pressures below atmospheric conditions and thermal temperatures near that of ambient temperatures [16]. This results in gas centrifuge technology having a much lower electricity requirement when compared to gaseous diffusion, but it also reduces the amount of material that each machine can hold as compared to gaseous diffusion cells. Depending on the design and configuration

of each machine, a gas centrifuge can only process milligram to gram quantities ofUF_6 at any given time [12]. Because of this low amount of material throughput in each machine, a GCEP will require many more separation elements when compared to a GDP. Besides the economic benefits associated with gas centrifuges over gaseous diffusion, there is an operational flexibility associated with these machines. These machines operate independent with respect to each other inside a GCEP, and with a single cascade containing thousands of individual centrifuges, the loss of a single machine will not greatly affect the performance of the rest of the cascade. This is of course under the assumption of a single machine failure, but in reality when one machine fails it will often catastrophically fail and destroy surrounding machines. Nevertheless, these machines can be "replaced, exchanged, and retooled in a plug-and-play manner during GCEP operation without dramatically affecting the remainder of the operating enrichment cascade"[16]. This allows for greater operational flexibility when compared to the rigid gaseous diffusion cascade where gaseous diffusion cells can not be replaced without affecting the overall performance of the cascade. This flexibility cannot be matched by gaseous diffusion. This does not mean that there are no downsides to using gas centrifuge cascades. The development of economical gas centrifuges requires high rotational speeds and advanced materials with a high durability and strength while maintaining a low density. Because of the nature of these materials, they are often sought out for a variety of material science applications in the space of high strength-to-density ratios. This means that the material in question for a gas centrifuge are controlled by the Nuclear Suppliers Group (NSG) and the Zangger Committee [4]. As stated previously, the next disadvantage of gas centrifuges is the material throughput compared to a single gas diffusion cell. This requires that a gas centrifuge cascade be made of many more elements when compared to a GDP cascade meeting the same desired end use of EUP. However, despite needing many more machines, the economic costs for operating a centrifuge cascade will still be lower than that of an equal gaseous diffusion cascade.

2.3 What is a Centrifuge Cascade

Because the individual separation of a single centrifuge or gas diffusion cell is very low, they must be plumbed together in series to reach a desired enrichment levels. Gas diffusion is a 1:1:1 ratio between the individual cell:stage:cascade meaning that there is only one cell per stage with a width equal to that a prescribed by ideal cascade theory. And there is one single massive cascade used to meet the desired EUP and product rate. However, there is more than stage in a GDP so the 1:1:1 ratio is really one cell per stage, as many stages as needed to get to desired EUP, and one cascade per GDP. A gas centrifuge cascade is a little different. This is because each machines throughput is lower than that of a gas diffusion cell. Therefore, they must be plumbed together in both series, one stage passing material to the next, and parallel, multiple centrifuges in a single stage. These cascades have defining characteristics such as their height, how many stages are in the cascade, the width, how many machines are in each stage, and the overall cut, the ratio of product to feed of the cascade. Each stage contains its own cut values which determine what amount of material is being passed to the product versus tails of a single stage. The cascading configuration means that for a given stage (n) there will be some amount of material entering this stage from stage (n-1) and (n+1). This re-circulation of material between stages is denoted as the hydraulic reflux of the cascade. This process of recirculating material occurs at every stage inside the cascade. For a two-component system such as natural uranium feedstock, the mass fraction of the U^{235} will be enriched by the square root of the stage's two-component separation factor as seen in equation 2.1.

$$X_{235n} = X_{235n-1} * \sqrt{\alpha_{mkn-1}} \tag{2.1}$$

Where α_{mk} is the separation factor associated with a two component system such as U^{235} to U^{238} and X_{235n} is the mass fraction of U-235 at stage (n). For the tails depletion, the mass fraction of U^{235} is depleted by $1/\sqrt{\alpha_{mk}}$. This material then gets passed back and forth between stages in a "cascading" fashion until the fully enriched material passes out the top of the cascade and fully depleted material is passed out of the bottom. This process can be seen in figure B.6. Additionally, each stage will suffer from both mixing and shaping losses.

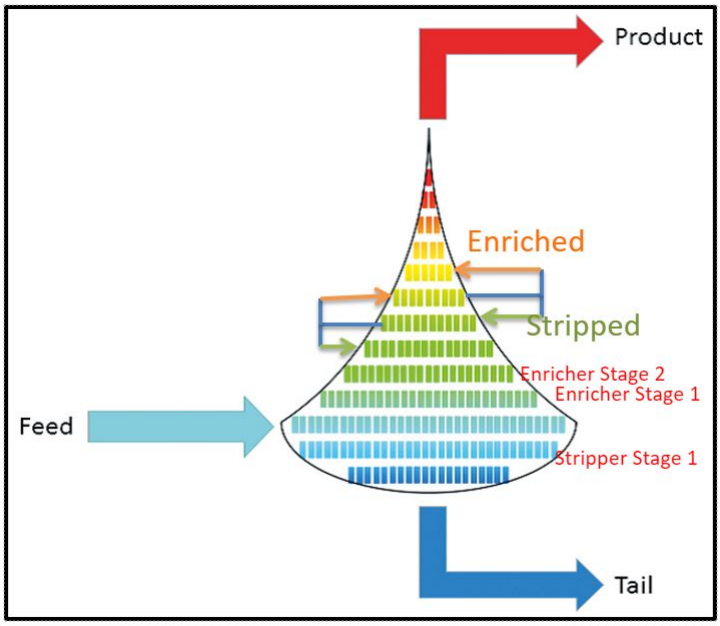


Figure 2.1: Overall design and operation of an enrichment cascade

Mixing losses occur when the product stream's assay of stage (n) does not match the tails stream's assay of stage (n+1). Shaping losses occur when the integer number of machines in a real cascade does not match what ideal cascade theory would dictate. In other words, ideal cascade theory may dictate that an ideal cascade would have 4.5 machines at stage (n) but in reality an operator can only use either 4 or 5 machines. This difference between the ideal prescription and reality is what creates shaping losses and can be seen in figure 2.2.

2.4 Current Cascade Methodologies

Although the work of this study is to primarily recreate the findings of the original NPACC under Dr. David Vermillion for his PhD dissertation, it is important to understand the origins of previous cascade analysis methodologies to gain a better understanding of how the original NPACC and newly developed NPACC-X improve over these methods. These previous modeling techniques have been primarily focused on understanding the separation mechanisms of a single centrifuge. They attempt to quantify the complex physical processes inside a centrifuge and how the design of a of a centrifuge affects the hydrodynamic and isotopic response of the processed gas as it passes through the

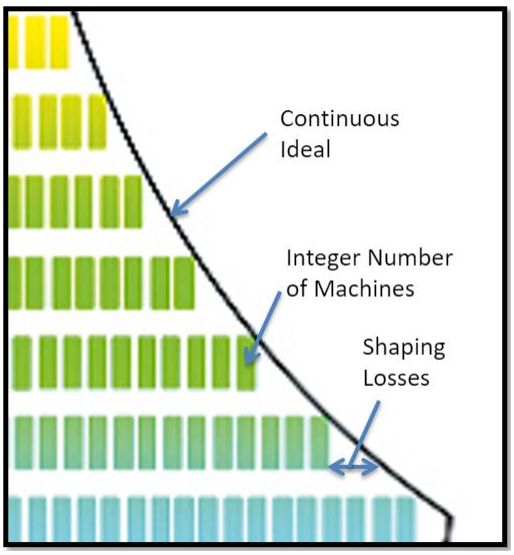


Figure 2.2: The difference between the continuous ideal and real world implementation of centrifuges creates shaping losses

machine. These efforts of previous centrifuge modeling resulted in creating performance maps of a single centrifuge design. These performance maps relate the centrifuge design and varying feed rates to a variable two-component separation factor and a SWU value to the given feed rate. The purpose of this study is not to dive into an analytical or numerical estimation of centrifuge performance, but rather it will use these previously created performance maps to gain a better understanding of the overall centrifuge cascade as it operates in a steady state condition. From a nonproliferation standpoint, understanding how all these centrifuges operate in conjunction with each other in a cascade is a much more important problem to solve because of the lack of proliferation potential of a single machine. It is currently believed that traditional cascade theory is good enough for the estimation of an overall enrichment cascade; however, Dr. Vermillion proposes that the overall lack of simulation and modeling precision does not lie with the single centrifuge but rather with the overall centrifuge cascade. This is because the overall performance of a single machine pales in comparison to the performance of the cascade when the cascade is "allowed to operate for a long enough duration of time to reach steady-state isotope separation conditions" [16].

2.4.1 Black Box

Black box analysis is the highest-level understanding of a single GCEP that nonproliferation analysits can operate on. It uses simply mass, isotope, and energy balance equations to determine the overall separation capacity of a single cascade or GCEP. In essence, it draws a "black box" around the entire facility and looks at the material entering and exiting the facility to make boilerplate estimations for SWU and capabilities of a given cascade. However, this method requires a great amount of material accountability to be of use as the feed rate, product rate, tails rate, feed assay, product assay, and tails assay must all be known in order to get an accurate answer. This method does not provide internal characteristics of a cascade such as machine type, number of enriching or stripping stages, or number of machines necessary for each stage of the cascade.

2.4.2 Ideal Cascade Theory

This method was developed during the Manhattan Project on the gaseous diffusion plants of the time. It analytically solves for the ideal cascade configurations based on certain assumptions of the enrichment technology in question[3]. These include symmetric separation, invariable cuts, invariable alphas, and that the real cascade will be perfectly tailored to an ideal cascade. This methodology worked well for gaseous diffusion when these assumptions could be held true. However, gas centrifuge technology does not adhere to these assumptions and have variable separation factors, cuts, asymmetric separation, and the stages cannot be perfectly tailored to ideal cascade theory.

2.4.3 MSTAR

This methodology was developed by Ed Von Halle at ORNL in 1987. It operates on a "Matched abundance ratio" whereby the mixing losses between stages are minimized by attempting to keep the product assay of stage (n) equal to the tails assay of stage (n+1) and so forth [6] [8]. This methodology allowed for multi-component analysis of isotopes in a centrifuge cascade. It is computationally fast due to its analytical derivations of isotopic gradients through the cascade and computationally applies ideal cascade theory

to each stage of the cascade. It utilizes a theoretical middle component (M*) to balance the material separation around. However, how this value is related to actual plant operation is unknown in the open-source. Although this represents the current best available cascade methodology, it still has some downsides. This method assumes constant separation factors whereas centrifuges have variable separation factors based on feed rate. The user must know the height of the cascade to make an accurate assessment and hydraulic performances are inaccurate due to the inability to quantify reflux. This method performs better when cascades are of sufficient size to simulate ideality [16]. Therefore, this method would be bad for small cascades with large separating elements.

Chapter 3

NPACC-X Methodology versus Original NPACC

This chapter will cover the overall methodology of the NPACC-X program developed in this study along with its predecessor, NPACC. This is because NPACC-X is derived from an early version of NPACC that was a first attempt at understanding two component separation. This results in the overall differences in the program lying in both the hydraulic reflux and multi-component separation due to the overall multi-component separation of a cascade affecting its internal reflux of material via the introduction of increased mixing losses.

The initial version of the two component NPACC primarily contained methods for accounting for internal mixing losses of a two-component mixture along with the calculation of separation factors for Rome and Iguacu machines assuming a two-component feedstock. This model operated by numerically following the mass and enrichment of the feedstock as it travels from stage-to-stage inside a cascade. Initially, the cascade is fed an enormous amount of feedstock to ensure that the initial cascade closely matches ideality. Then this mass is followed as the program builds the height of the cascade in order to reach the desired enrichment level for the system. Once the height has been established, then the cascade is further iterated over until a steady state configuration of the cascade has been established. At the end of this process, a cascade that is operating in steady state has been built that matches the desired enrichment level of the cascade but will probably be producing too much

product material. Therefore, the overall cascade cut, ratio of product to feed, can be used to make a better guess for what the feed rate for the cascade should be, given that the overall height of the cascade does not change. This newly guessed feed rate is used to iterate over the cascade height until a steady state width has been established again. Then this program will check how closely the new product rate matches the desired product rate, and using this information, it will rank how well this cascade met the desired EUP. This building of steady state cascades is performed several times while stochastically varying the feed rate until the pseudo-simulated annealing algorithm determines the "best fit" cascade for a given EUP.

This overall, original NPACC program workflow can be seen in 3.1.

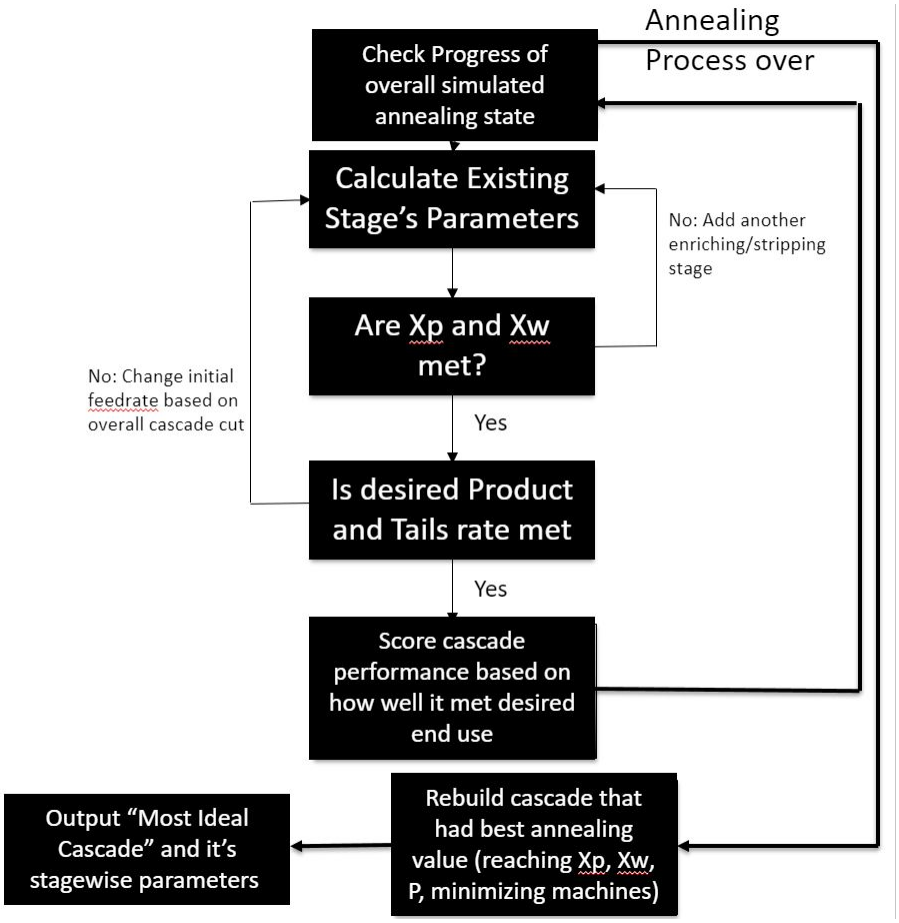


Figure 3.1: NPACC-X and NPACC's original cascade analysis methodology

This methodology utilized a numerical solution to the design of cascade shapes thus circumventing the need for an analytical solution to the overall cascade shape or isotopic gradient inside the cascade. Additionally, it numerically accounts for mixing losses of U^{235} and U^{238} by tracking the physical amount of mass present of each isotope inside each stage and calculating how much mass of each isotope is being moved between stages. In order to address the issue of shaping losses, this program dynamically calculates the stagewise overall isotopic separation factor by taking the stage machine's average feed rate and using performance maps from "Semi-Empirical Method for Developing a Centrifuge Performance Map" to determine this separation factor on a single stagewise basis [13]. Once the program has completed, it results in a stage-by-stage understanding of the cascade's physical parameters while not having to meet the previous assumptions under ideal cascade theory such as no mixing or shaping losses. This will more closely match the reality of actual GCEP operation and bridges the gap between empirical cascade data that was not matching cascade modeling data. The version that NPACC-X started from was the original workflow in figure 3.1; however, in order to address multi-component separation various functionalities must be added to this original codebase. Specifically, the ability to track minor isotopic separation factors, cuts, and the overall isotopic composition of the stagewise feedstock would have to be added to address the problem of multi-component separation.

3.1 NPACC-X Methodology and Differences from NPACC

In order to address the issue of multi-component separation, the underlying programmatic procedure used in NPACC remains the same while additional variables must be added to the program to track the minor isotopic separation. This subsection will be devoted to explaining the NPACC-X methodology while covering the differences on the intra-stage, inter-stage, and overall cascade calculations between NPACC and NPACC-X. Firstly, it is important to understand what is being calculated on a stagewise basis inside of NPACC-X. This parameters include U^{235} mass fraction, stagewise feed rate (kgUF6/yr), number of machines in each stage, single machine average feed rate (mg/s), overall separation

factor (α_{mk}), overall stage cut (θ), separative capacity (SWU/yr), stage product rate, stage tails rate, the mass fraction of each minor isotope, overall average heavy isotopes molecular weight (MW_{heavy}), and the overall average light isotopes molecular weight(MW_{light}). This results in 16 different parameters being calculated at each stage. These 16 parameters are calculated on a single stage basis and then the program moves one stage up or down inside the cascade and recalculates these parameters based on the parameters from stage n+1 and n-1. For clarities sake, each parameter's stagewise equation will be given to show what is being calculated and how the immediate surrounding stages affect a single stage's characteristics. The first variable calculated in each stage is its U^{235} mass fraction. This is calculated via equation 7 whereby j = [1,2,3,4,5,6] and corresponds to the isotopes [U^{235}, U^{232}, U^{233}, U^{234}, U^{236}, U^{238}] respectively.

$$X_{j_n} = \frac{\dot{P}_{n-1} * X_{j_{n-1}} * \alpha_{mk}^{\frac{MW_{heavy}-MW_j}{MW_{heavy}-MW_{light}}} + \dot{T}_{n+1} * \frac{X_{j_{n+1}}}{\alpha_{mk}^{\frac{MW_{heavy}-MW_j}{MW_{heavy}-MW_{light}}}}}{\dot{P}_{n-1} + \dot{T}_{n+1}} \tag{3.1}$$

From this equation, the single stage's X_{235} is calculated using the previous stage's product rate and multiplying it by the mass fraction of the enriched U^{235}. This results in a calculated amount of mass of U^{235} entering this stage from the previous stage's product stream. This value is added to the amount of U^{235} mass coming in from the next stage's tails stream. Then this total amount of U^{235} mass is divided by the total amount of mass entering the stage from stages n+1 and n-1. This results in this specific stage's U_235 mass fraction. Next is the stagewise feed rate, this is a simple calculation whereby $\dot{F}_n = \dot{P}_{n-1} + \dot{T}_{n+1}$. This holds true except for in the edge cases such as the feed stage or final stages in the cascade. At the feed stage $\dot{F}_n = \dot{P}_{n-1} + \dot{T}_{n+1} + \dot{F}_{cascadeFR}$ and if at the top of the cascade, $\dot{F}_n = \dot{P}_{n-1}$, or at the bottom of the cascade, $\dot{F}_n = \dot{T}_{n+1}$. The presence or lack thereof of feed streams must be accounted for all variables. In other words, every time the program is at the feed stage or edge stages of a cascade, the isotopic vectors must include these additional feed streams or lack of additional feed streams. Then, the program will calculate the ideal number of centrifuges in this given stage using the

stages feed rate $\dot{F}_n$. The number of machines inside a single stage is simply the total feed rate to the stage F_n divided by the ideal machine feed rate (L_{opt}). This value is rounded down to the next integer except in the case where rounding down would equal to zero machines, in that case it is rounded up to one. This program rounds down across all stages of a cascade because the minimum number of machines in a stage to reach a desired EUP is the most economic solution.

After the number of machines in a stage is calculated, the program will calculate the single machine's average feed rate. The Average Machine Feed rate = $\frac{F_n}{Machines_n}$. This average single-machine feed rate is then used to calculate α_{mk} by going to a performance map and looking up what α_{mk} would be for the given machine feed rate(Woods). Next, the stagewise overall cut of the centrifuge is calculated using the following equation:

$$\theta_{mk} = \frac{(1 + \sqrt{\alpha_{mk}^{\frac{MW_{heavy} - MW_j}{MW_{heavy} - MW_{light}}}} - 1) * X_{235_n}}{1 + \sqrt{\alpha_{mk}^{\frac{MW_{heavy} - MW_{235}}{MW_{heavy} - MW_{light}}}}} \tag{3.2}$$

This equation is the same as the one used in Dr. Vermillion's dissertation except for the fact that it raises the α_{mk} to the power of the differences in molecular weights between the average heavy isotopic weights, average light isotopic weights, and the molecular weight of U_{235}. The addition of the exponential term to $\alpha_m k$ was incorporated to attempt to simulate how the cut will change due to the change in the overall isotopic composition.

The SWU/yr term is calculated from the performance map of the machine which results in a SWU/yr/machine. This is then multiplied by the number of machines in the given stage to result in a SWU/yr/stage. However, Dr. Vermillion has noted that the calculated of SWU/yr/machine from Wood's performance maps may be inaccurate, but for consistencies sake it has been left in the code.

The stagewise product rate can be calculated by taking the overall stage cut (θ_n) and multiplying it by the stage feed rate ($\dot{P}_n = \theta_n * \dot{F}_n$). Conversely, the stagewise tails rate is simply $\dot{T}_n = \frac{1}{\theta} * \dot{F}_n$.

Each minor isotope's mass fraction can be calculated using the same equation as 7 whereby the MW_{235} is substituted for the molecular weight of the minor isotope in question (e.g. MW_{232}, MW_{233}...). Here lies a potential problem area for this program because rather than depleting or enriching U^{238} in the same way as the minor isotopes or key isotope, U^{238}'s mass fraction is calculated as the remaining amount of mass left over after all other minor isotopes new enrichment values have been calculated; whereas before, the stagewise U^{238} concentration would be calculated as the inverse of the U^{235} concentration due to the original theory being founded in a two component system. In other words, since there were only two components, as one component was enriched by a certain amount, the other component had to be depleted by an equal amount to maintain mass balance. This potential inability to quantify U^{238} depletion will be covered in Chapter 4. Lastly, the stagewise average heavy and light isotopes molecular weights are calculated by first classifying what counts as a "heavy" or "light" isotope. For this study, anything lighter than U^{235} is considered to be a light isotope while anything heavier than U^{238} is considered a heavy isotope. For the case of U^{236}, it is classified as being 2/3 heavy isotope and 1/3 light isotope. Therefore, the equations for calculating average molecular weights would look like:

$$MW_{heavy_n} = \frac{X_{238_n} * MW_{238} + (2/3) * X_{236_n} * MW_{236}}{X_{238_n} + (2/3) * X_{236_n}} \tag{3.3}$$

And,

$$MW_{light_n} = \frac{X_{232_n} * MW_{232} + X_{233_n} * MW_{233} + X_{234_n} * MW_{234} + X_{235_n} * MW_{235} + (1/3) * X_{236_n} * MW_{236}}{X_{232_n} + X_{233_n} + X_{234_n} + X_{235_n} + (1/3) * X_{236_n}} \tag{3.4}$$

These are all the calculations being performed on a single-stage basis. These calculations are performed thousands of times in series as the program moves the material up and down the

cascade until it reaches a steady state configuration where these variables are no longer changing due to the feed of the cascade. The differences between the original NPACC and NPACC-X within these parameters are primarily in the introduction of MW_{heavy}, MW_{light}, raising α_{mk} to the differences between these weights, the incorporation of each isotopes mass fraction on a stagewise basis, the change of overall cascade cut to include the stage's isotopic vector, and a stagewise isotopic balance function to ensure the program maintains isotopic balance. On the inter-stage level, the difference between NPACC and NPACC-X include the introduction of minor isotopes to the overall mixing losses of a stage. This means that each stage must include how the minor isotopes presence changes each isotopes mass fraction. This can be performed by simply including these minor isotopic vectors when you are calculating a single stage's isotopic mass fractions. Simply put, this program makes sure to account for how the presence of the minor isotopes affects the key isotopes mass fraction by including the amount of mass entering a stage from these minor isotopes. Macroscopically, NPACC-X does not vary much from its predecessor in terms of the overall workflow. The key differences being the introduction of another check that allows the cascade "wiggle room" for when it's close to a solution so that it can add or subtract a stage if under extreme non-ideal situations. This was because the original NPACC would sometimes struggle to find a solution when performing highly unideal calculations of cascades such as HEU production with limited machines. For example, when Rome machines are underfed, their separation factors skyrocket. So, if a cascade is trying to reach HEU production with a low throughput the shaping losses will create a large amount of varying between two cascades that may only differ by one stage. Often, the original NPACC would struggle to find a solution that reached the desired EUP while also reaching the desired material throughput. This functionality was added so that the program could more quickly and easily vary the cascade shape by small amounts to see if the tweaks resulted in a steady state solution that reached the desired end use.

3.2 Case Studies and Motivations

In order to benchmark this program to something existing in the real world, the same case studies from Dr. Vermillion's dissertation will be re-evaluated using NPACC-X. These cases will be covered in brevity but understanding the motivation behind picking these cases is important to the evaluation of NPACC-X as a cascade analysis tool.

The first case studied is an impractically ideal, large cascade supporting the continuous refueling needs of a 65 pressurized water reactor (PWR) fleet. This was chosen to simulate a cascade that was so large that the mixing and shaping losses present in the cascade would be negligible compared to the overall mass throughput of the system. The gross average EUP demand associated with this end use is 1,778,125 kgU/yr %5 U^{235} [16]. Realistically, multiple GCEPs operating in parallel would be utilized to reach this end goal; however, in both this study and Dr. Vermillion's dissertation, it serves as a benchmarking tool only.

The second case study is one to determine the differences in cascade analysis methodologies on a cascade that would more closely simulate reality. This would be the design of a cascade to support 1/50th the need of a continuously fueled VVER-1000 unit. This unit was chosen for two reasons, the first being that the VVER-1000 is a popular PWR design operated throughout the world and is associated with the lowest estimated equilibrium fuel consumption rate [16]. The reason that the cascade supports only 1/50th the total need of the reactor is based on the assumption that rather than one large cascade supply the needs of a single reactor, 50 parallel cascades would be built to meet this desired material throughput [7]. For continuous operation, this results in a need of 412.92 kgU/yr %5 U^{235}. This case study will cover the differences in cascade analysis techniques and how ideal realistic compact cascades are.

The third case study analyzes the purely peaceful centrifuge cascade requirements for meeting the EUP demand associated with a research reactor. Although research reactors do not warrant the building of a domestic enrichment program to fulfill their refueling needs, this case study is performed to analyze a cascade design that would produce high-duty LEU fuel to research reactors. This case study focuses on Australia's Opal research reactor

which is conservatively associated with refueling requirements of 73.37 kgU/yr %20 U^{235}. This represents the highest EUP demand associated with any LEU operating reactor in the world. This case study is provided to highlight the differences in predicting cascade size and separative performances for LEU research reactors.

The fourth and last case study focuses on NPACC-X's ability to characterize small, highly unideal cascades with varying feedstocks. Therefore, the most appropriate reactor would be ORNL's HFIR which requires approximately 121.16 kgU/yr %93.1 U^{235} for continuous refueling and operation. This case study is used to highlight what a centrifuge cascade would look like for the production of WGU and how these unideal cascades can vary from classical cascade theory.

Chapter 4

Results and Differences of Case Studies

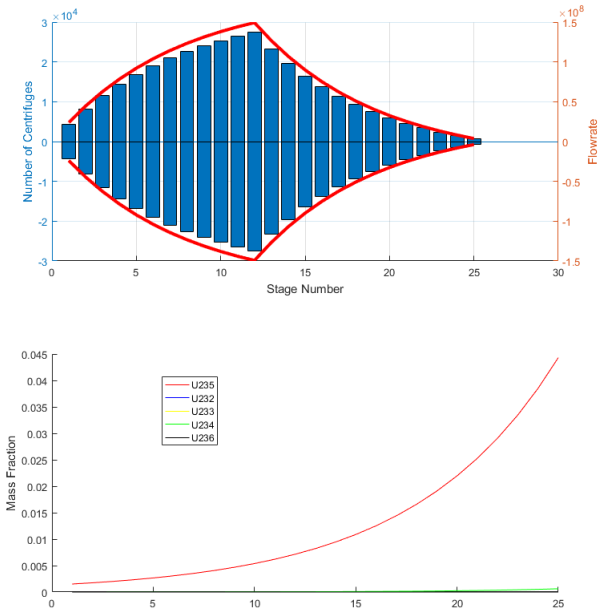
This chapter will revolve around presenting the results from the four case studies and discussing any differences between the findings of the original NPACC versus the newly developed NPACC-X. Unfortunately, this author was never able to get a digital copy of the underlying data found in Dr. Vermillion's dissertation so the data provided by NPACC-X will be compared to the numerical results found in Dr. Vermillion's study. This means that there will be a lack of figures provided by the original NPACC; however, most of the results will still be able to be covered despite the lack of visual information surrounding the original NPACC. Each case study will include both centrifuge designs, Rome and Iguacu, along with two different feedstocks, natural uranium and reprocessed uranium. This is to show how different centrifuge designs will have different effects upon overall cascade shape and what level of losses are introduced into the system.

4.1 Case 1: 65 PWRs with continuous refueling

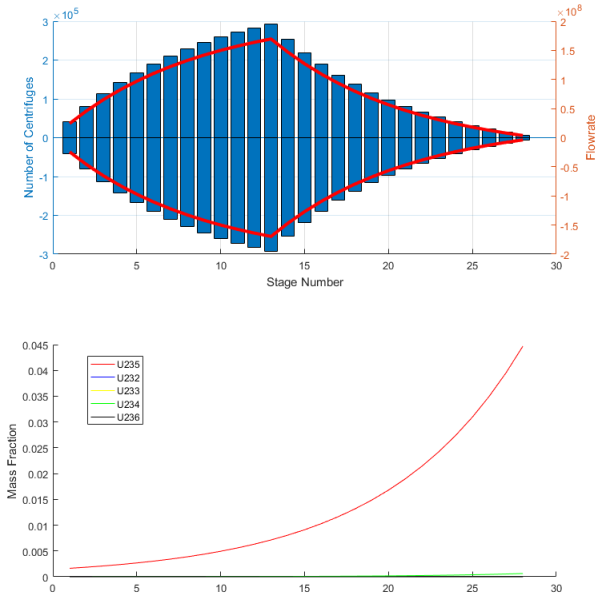
The goal of this case was to present an impractically large and ideal cascade for comparison to the original cascade analysis methodologies such as Black Box Analysis, MSTAR, and NPACC. Because of the size of the width of this cascade, NPACC can easily find a solution to

reach %5 enriched U^{235} for the PWR fleet within a matter of seconds. The first cascade profile's shown are for a natural uranium feedstock given both the Rome and Iguacu machines.

From figure 4.1b it can be seen that a cascade made entirely from Iguacu centrifuges will need more machines as compared to its larger counterpart the Rome. Additionally, an Iguacu cascade will need an additional three stages in order to meet the desired EUP demand. This is due to lower separation factor associated with the Iguacu machines that results in a need for more enriching stages to reach a similar assay enrichment. However, this still varies from the original NPACC that dictates that a Rome cascade would only need 21 stages to reach its desired EUP demand as compared to NPACC-X's 25 stages. MSTAR also agrees with the original NPACC in reaching the desired enrichment level in 21 stages too. Additionally, NPACC-X has a lower hydraulic reflux than its predecessor and finds that an optimal cascade would have 341,358 machines as compared to NPACC's 407,233 machines. This underestimation of hydraulic reflux remains constant across all cases as compared to the original NPACC. However, the individual isotopic separation factors, and their subsequent isotopic cuts, are different between NPACC and NPACC-X. NPACC dictates that the U^{235} separation factor remains constant at around 1.15 whereas NPACC-X finds a constant separation factor of around 1.32 for the Rome machines. This discrepancy between constant separation factors points to where the first issue of this code may lie. Because the Rome and Iguacu machines are both theoretical, they cannot have their separation factors validated for a given stage feed rate. Although it is unclear which version of the code contains the correct version of the centrifuges' performance maps, it can be certain that they must vary in some way between the two codes. This results in a different number of stages needed to reach the desired enrichment level along with changing the cascade width due to each stage's cut being determined by its separation factor. This could be one source of the differences in hydraulic reflux between the two codebases. Next, the same 65 PWR fleet is fueled with a single cascade being fed reprocessed uranium. The presence of the minor isotopes found in reprocessed uranium should affect the overall cascade shape due to an increased amount of mixing and shaping losses. The reprocessed

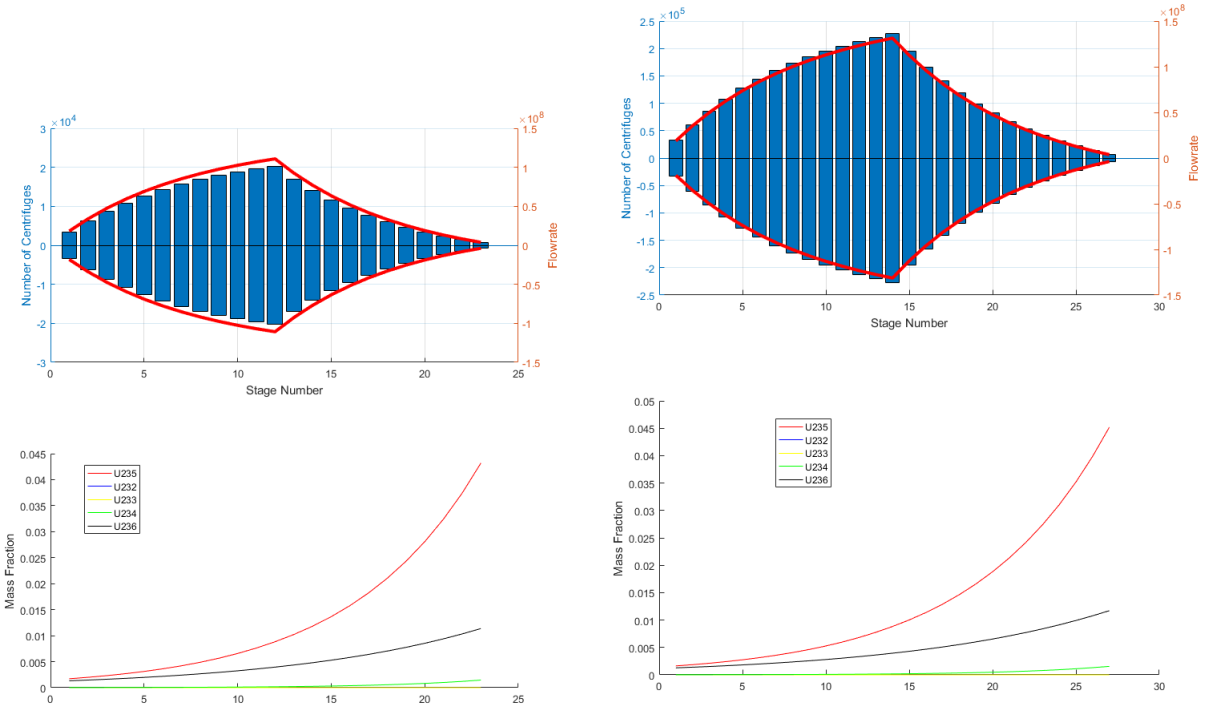


(a) Rome



(b) Iguacu

Figure 4.1: Rome and Iguacu cascades fed with natural uranium for a 65 PWR fleet



(a) Rome **(b)** Iguacu

Figure 4.2: Reprocessed Uranium cascade for 65 PWR fleet

uranium cascades for Rome and Iguacu centrifuge cascades can be found in figure 4.2a and figure 4.2b.

While there remain some similarities between the NU feedstock cascade and RepU feedstock cascade, there are some notable differences. Specifically, both the Rome and Iguacu enrichment cascades need fewer stages to reach the desired enrichment level as compared to their natural uranium counterparts. This was unexpected as the presence of minor isotopes should introduce additional mixing losses and hamper the separation of U^{235} to U^{238}. However, the reduction in cascade height may be due to the presence of U^{236} inside the cascade which can act as a partial heavy isotope further bolstering the amount of heavy material present inside each machine. This increase in heavy isotopes in the machine could hypothetically raise the separation factor of light isotopes which would result in a shorter cascade height. However, the hydraulic reflux inside the cascade remains lower than what the original NPACC predicted. The original NPACC predicted that one would need 299,665

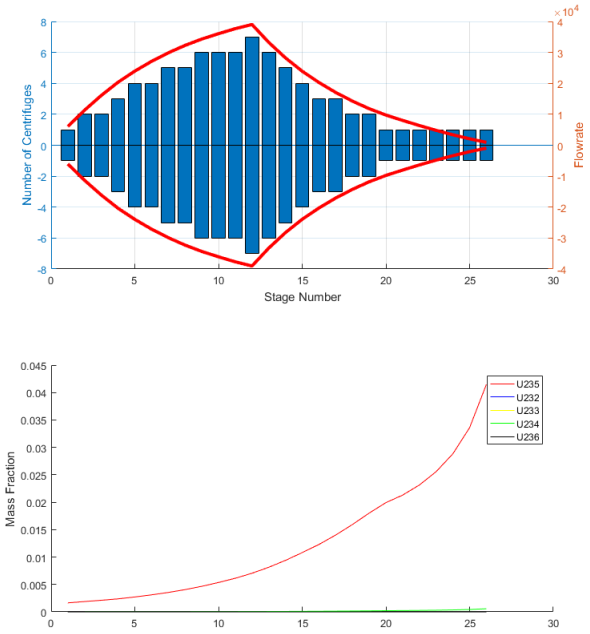
Rome machines to fuel 65 PWRs whereas NPACC-X predicts that one would need 243,916 Rome machines to achieve the same result. This still points to there being a discrepancy between NPACC and NPACC-X in the performance maps and characteristics of the Rome and Iguacu machines. However, minor isotopic composition at the product stage remains similar between NPACC and NPACC-X. Here, NPACC finds that there would be 0.00156, 0.00997, 3.68E-08 weight percent U^{234}, U^{236}, and U^{232} respectively. Compare this to NPACC-X's 0.00146, 0.0113, and 3.48E-08 and it is found that there is a 6.4%, 13.34 %, and 5.4% difference between each model's prediction of the minor uranium isotopic weight percentage. This is much closer than expected especially when compared to the nearly 20-30

4.2 Case Study 2: 1/50th VVER-1000

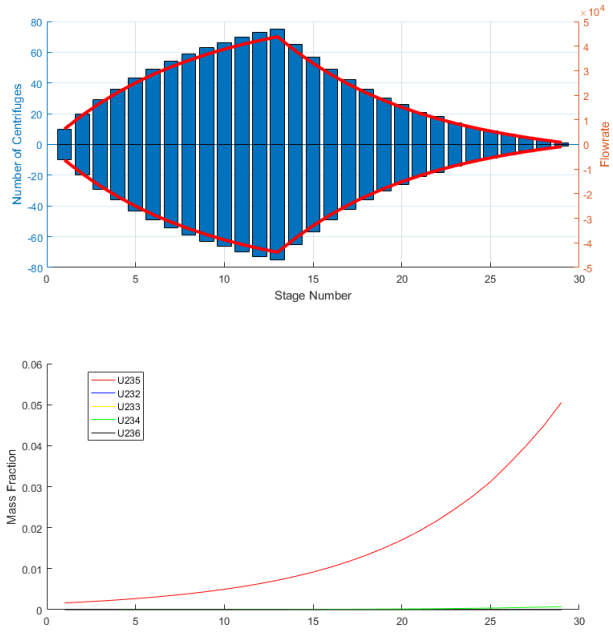
This cascade serves as the smallest, realistic cascade that could be found in the world in order to analyze how ideal these cascades are and how they respond to the introduction of multi-component analysis. With a product throughput of 412.92 kgU/year %5 enriched, these cascades have a relatively small throughput while still reaching a real-world enrichment level used for peaceful purposes. First it is important to understand what a natural uranium cascade would look like to meet this EUP demand. This can be seen in figures 4.3a and 4.3b for natural uranium feedstocks0.

Here, it is seen that both the Iguacu and Rome cascades both exhibit some forms of non-ideality in their cascade performance. This is due to the shaping losses that occur inside the cascade as each machine begins to be slightly over or under fed as the cascade reaches stages with only one machine inside each stage. From figures 4.3a and 4.3b it can be seen that this point of nonideality occurs around stage 20 for the Rome cascade whereas the Iguacu cascade does not suffer much from the mixing losses and shows a smooth enrichment curve to %5 EUP.

This case shows NPACC's ability to quantify shaping losses inside of non-ideal cascades and how machine performance specifications can determine the ideality of a cascade between two different enrichment machines for the same desired end use. This example

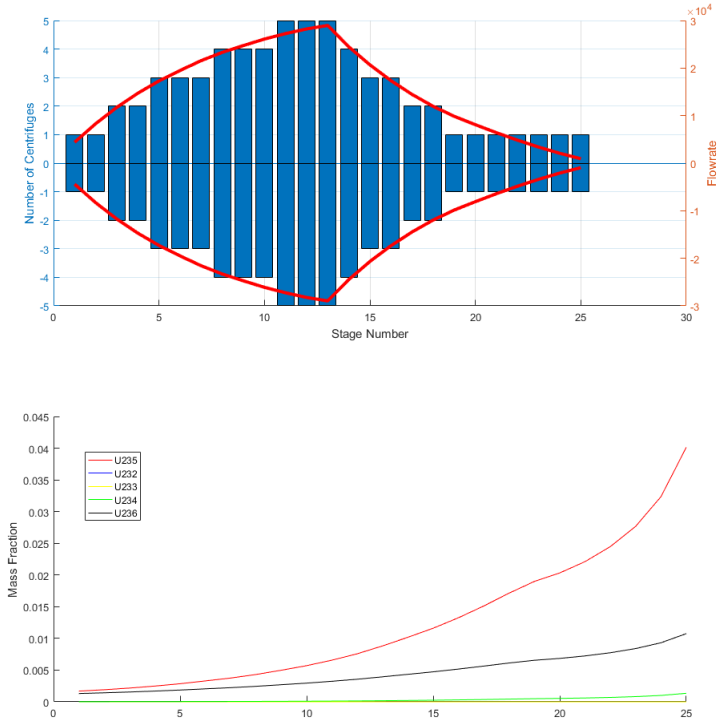


(a) Rome

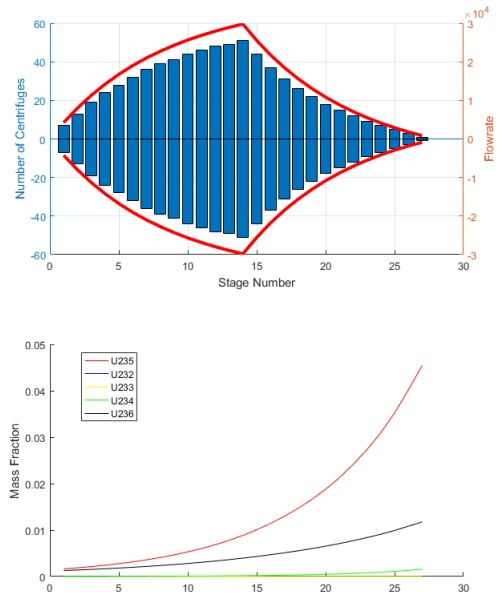


(b) Iguacu

Figure 4.3: Natural Uranium cascades for 1/50th VVER-1000



(a) Rome



(b) Iguacu

Figure 4.4: Reprocessed Uranium cascades for 1/50th VVER-1000

shows one of the largest benefits of NPACC as its ability to quantify shaping and mixing losses gives more insight into minor isotopic enrichment through cascades that differ from purely ideal cascade theory. The Iguacu cascade more closely mimics a purely ideal cascade as the material holdup and throughput of this machine is lower than that of the Rome machine. Therefore, for the same stagewise flowrates to meet some EUP demand, the Iguacu machines will suffer less shaping losses as the difference between what is recommended by ideal cascade theory and reality is minimized.

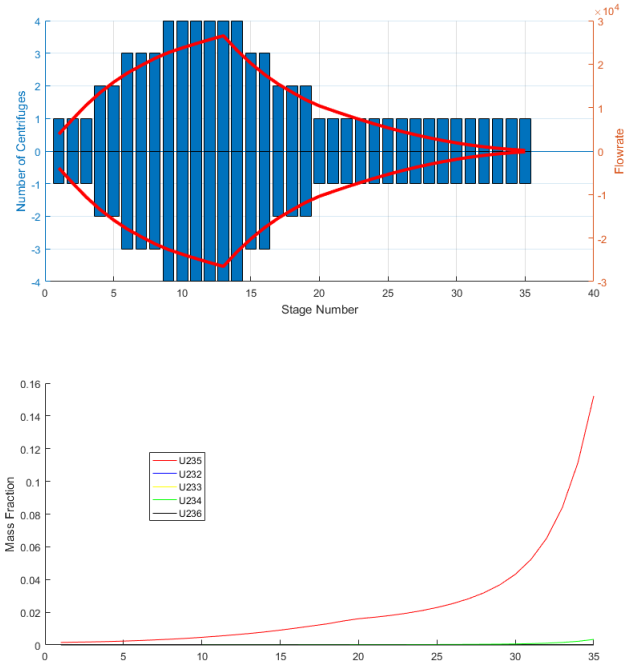
Additionally, the difference between the reprocessed uranium feedstock cascade and natural uranium cascade is of concern for this case study. Between figures 4.3a and 4.4a it can be seen that there are 15 enriching and 11 stripping stages for the natural uranium cascade whereas there is only 13 enriching and 12 stripping stages for the reprocessed uranium. Although the exact mechanisms behind this change in cascade shape are still unclear, it can be theorized that the increase in stripping stages and decrease in enriching stages of the reprocessed uranium cascade can be attributed to the increased presence of heavy isotopes inside the cascades feedstock vector. This is because the increase in heavy isotopic composition (i.e. U^{236}) will require additional stripping stages to help with the removal of these heavy isotopes whereas in the enriching portion of the cascade, the additional presence of the heavy isotopes actually helps to increase the separation of U^{235} as it has more heavy isotopes to "push on." This increase in stripping stages results in irregularities occurring from non-ideality to occur one stage lower inside the reprocessed uranium cascade as compared to the natural uranium cascade. This can be seen at stage 20 of the natural uranium cascade and stage 19 of the reprocessed uranium cascade.

4.3 Case Study 3: OPAL Reactor

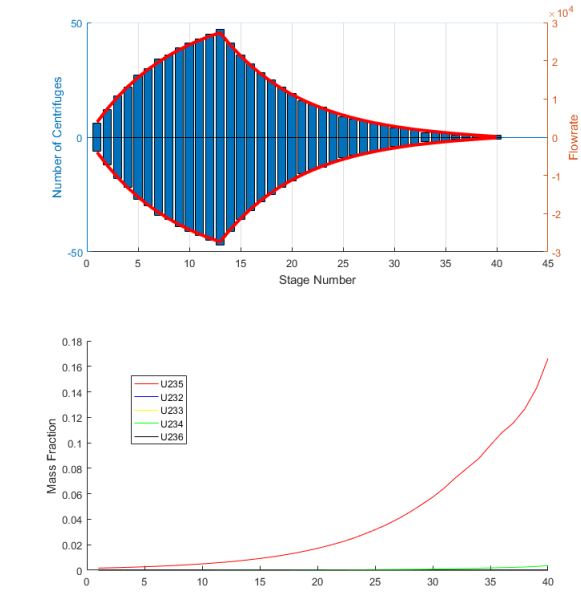
The OPAL research reactor is of concern in this study as it allows for the investigation of peaceful production of heavy-duty LEU fuel. This 20% EUP requires much more separative work than its %5 counterparts, and subsequently, it will require the cascade

to experience increased mixing and shaping losses as the material throughput is relatively low while the desired EUP is the highest for LEU production. The Rome and Iguacu cascades for natural and reprocessed uranium can be seen in 4.5a, 4.5b, 4.6a, 4.6b.

Interestingly, there is significant differences between the natural uranium Rome and Iguacu cascades. Specifically, the point of non-ideality for the Iguacu cascade does not occur until high up in the enrichment portion of the cascade, around stage 33. However, for the natural uranium fed Rome cascade, the first notable point of non-ideality occurs at stage 20. This is because in the Rome cascade there is a presence of a long chain of single machine stages, all of which are being underfed. This series of underfed Rome machines greatly increases the separation factor of the machine while reducing the overall separation capacity of the machine. This increase in separation factors of the machine results in the steady state isotopic curve of the Rome cascade to be shifted towards the heads of the cascade. Therefore, the point of non-ideality inside the Rome cascade begins much earlier compared to the Iguacu cascade as the shaping losses start to become more significant at earlier stages due to the stagewise material throughput compared to the overall machine throughput. Additionally, in the Rome cascade, from stage 20 onward it can be seen that there is only 1 Rome machine per stage which results in each of these stages suffering from increased mixing and shaping losses. This would point to smaller machines being better suited for heavy-duty LEU production when the overall material throughput of the cascade is relatively low. Comparing the reprocessed uranium cascades to the natural uranium cascades, the Rome and Iguacu cascade experiences a similar response to reprocessed uranium as it did in Case Study 2. For the natural uranium cascade, there are 27 enriching and 12 stripping stages; whereas, for the reprocessed uranium cascade, there are 25 enriching and 13 stripping stages. Again, the presence of the heavy isotopic composition in reprocessed uranium will dictate that there needs to be an additional stripping stage to deal with the presence of these heavy isotopes, but there can also be a reduction of the enriching stages as the U^{236} adds to the isotopic buoyancy of the U^{235}. This presence of the heavy isotopes also shifts the point of non-ideality inside both cascades down one stage in both cascades.

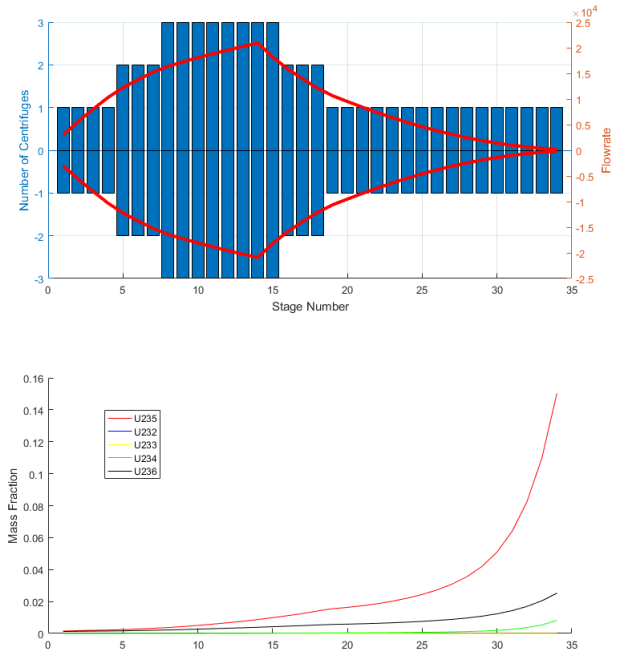


(a) Rome

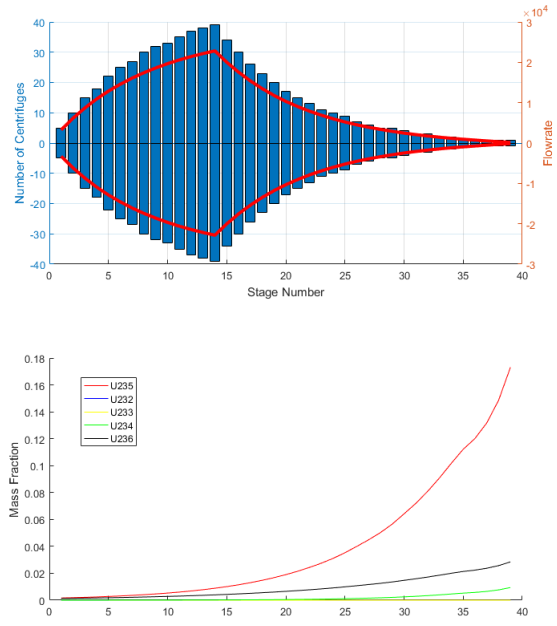


(b) Iguacu

Figure 4.5: Natural Uranium cascades for OPAL research reactor



(a) Rome



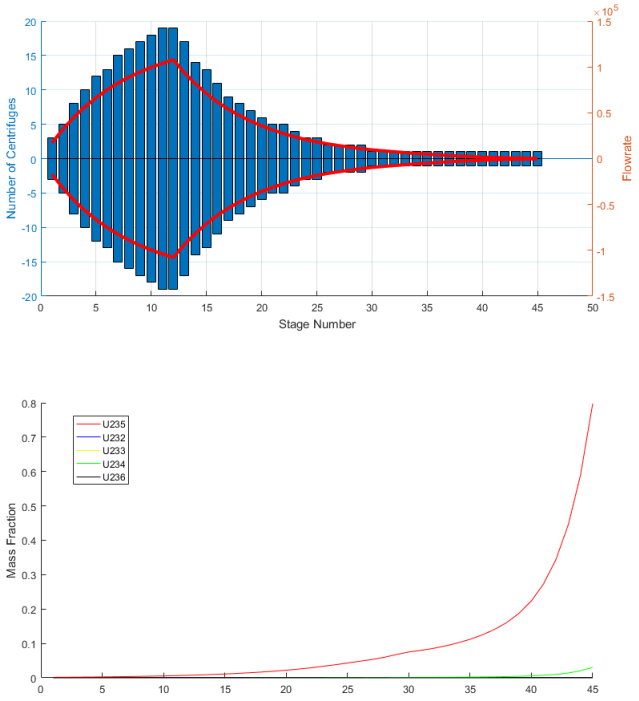
(b) Iguacu

Figure 4.6: Reprocessed Uranium cascades for OPAL research reactor

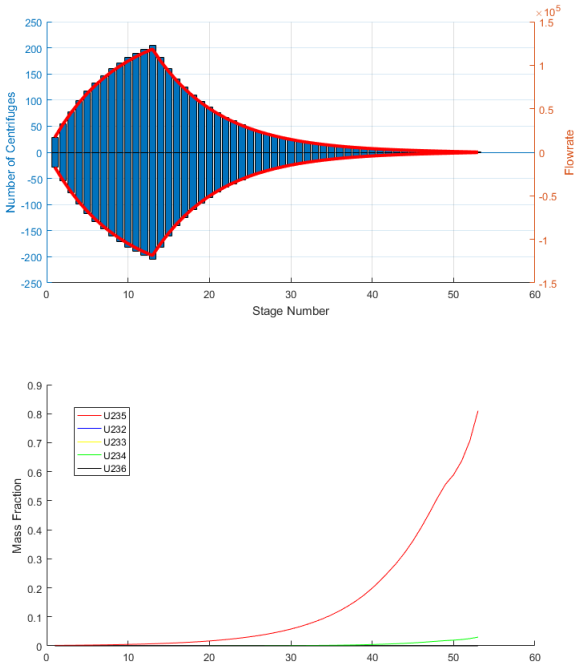
4.4 Case Study 4: ORNL's HFIR

This case study focuses around NPACC's ability to characterize HEU production cascades and what sort of non-idealities occur with a low material throughput and HEU production scenario. This case can give nonproliferation analysts insight into size, shape, and capabilities of WGU production cascades.

Similar to the OPAL research reactor, it can be seen in 4.7a and 4.7b that the point of non-ideality begins at the point where the required number of machines in a stage approaches one. Therefore, again it can be seen that for HEU production at a low material throughput the point of non-ideality occurs lower in the Rome cascade as compared to the Iguacu cascade. From the point of non-ideality onward, both cascades exhibit an exponential increase in U^{235} enrichment as these machines are underfed and their separation factors are increased. Interestingly however, the number of machines required to reach this EUP demand is only 284 Rome machines and 3,291 Iguacu machines. This is of importance as it demonstrates the capability of a potential proliferator to leverage a loss in separation capacity as these machines are underfed to reach to EUP levels demanded of WGU. This means with few Rome machines; this potential proliferator could intentionally underfeed these machines to increase their separation factor to reach %90 enriched uranium while sacrificing some amount of SWU on a stage-by-stage basis. The benefit of this model is that this increase in separation capacity comes with notable signatures in the isotopic gradient of the cascade. If non-proliferation analysts could take measurements at different points of the cascade, this non-ideal isotopic gradient could be discovered allowing the nonproliferation analysts to infer about the overall end use of this cascade. Interestingly, there is a similar pattern as case studies 1 and 2 between the natural uranium feedstock cascades and the reprocessed uranium cascades. The reprocessed uranium cascades tend to have additional stripping stages to account for the increased presence of heavy isotopes and fewer enriching stages as these heavy isotopes help to boost the separation factor of U^{235}. As the U^{234} is enriched simultaneously in the cascade, by the time U^{235} reaches 90% enriched the U^{236} and U^{234} mass fractions are roughly equal at the top of the cascade. This is because U^{234} starts at a naturally lower enrichment compared to the

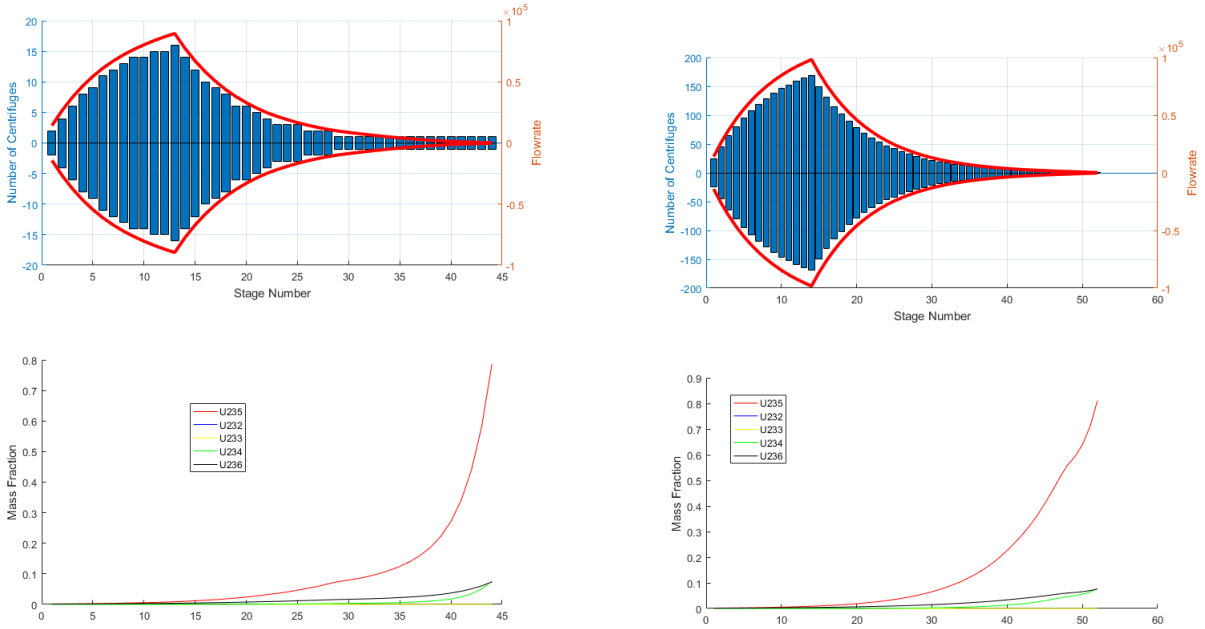


(a) Rome



(b) Iguacu

Figure 4.7: Natural Uranium cascades for HFIR research reactor



(a) Rome **(b)** Iguacu

Figure 4.8: Reprocessed Uranium cascades for HFIR research reactor

U^{236} but its separation factor is higher due to it being roughly 2 AMU lighter than U^{236}. This leads to another isotopic checkpoint for potential nonproliferation analysists as an inspector could measure the product's assay content and if the U^{234} levels match U^{236} it points to a potential proliferation scenario with reprocessed uranium. Despite the lack of U^{232} and U^{236} in a natural uranium cascade, the difference in the products concentration of U^{234} between HEU and LEU production can be seen with respect to 4.1a and 4.7a. Here, the U^{234} mass fractions in the %5 versus %90 enriched natural uranium cascades are 0.00062 and 0.0305 respectively. This means that for a nonproliferation analyst tasked with ensuring the prevention of proliferation of natural uranium cascades, measuring the products U^{234} concentration can give insight into the desired end use of a natural uranium cascade even without the presence of other minor isotopes from reprocessed uranium.

4.5 Differences in Case Studies:NPACC vs. NPACC-X

Firstly, it is important to reiterate that both NPACC and NPACC-X cannot be verified or validated to any existing cascade datasets. This is due to the nature of uranium enrichment cascades as their overall performance, shape, and machine characteristics are closely guarded by the operators and the release of this information would be of great proliferation concern. NPACC-X is still benchmarked to the original NPACC as it is an attempt to recreate its predecessor. Further assay, shape, and performance analysis of these case studies as compared to the original NPACC can be found in Appendix B. Across all case studies, NPACC-X underestimated the amount of hydraulic reflux inside the cascade and thus underestimated the number of machines inside a cascade as compared to its NPACC counterpart. After presenting this work to Dr. Vermillion, it was theorized that there was a difference in the performance maps used by the original NPACC versus NPACC-X. For example, in case study 1, the separation factors for both NPACC and NPACC-X remain constant throughout the cascade due to its large size and highly ideal nature. However, NPACC-X found that the separation factor of the U^{235} was around 1.32 whereas NPACC found it to be around 1.15 for a Rome machine cascade. Because these cascades are highly ideal, it points to a difference in the actual performance maps used by the two programs as a source of these discrepancies. This difference in separation factors also changes the overall stagewise cut as the cut is derived from the overall stage separation factor. Therefore, this change in separation factor and cut could be the reason why there is less overall hydraulic reflux inside the cascade. These performance maps also dictate the ideal material holdup inside each machine; thus, if there is a change to the optimal feed rate of the machine, then there will a change in the ideal number of machines per stage.

NPACC-X also handles the individual isotopic separations factors differently than NPACC. Although the exact mechanisms by which the minor isotopic separation factors are calculated inside NPACC are unknown, it can be theorized that it is along the lines of equation 1 in Appendix A. In NPACC-X, the minor isotopic separation factors use the same equation; however, the average major and minor isotopic weights are

dynamically calculated on a stage-by-stage basis. Then, each stage has an additional isotopic balance loop to ensure that all minor isotopic compositions add up to 1. Dr. Vermillion has stated that there is no stagewise isotopic balancing, but rather, there is an overall cascade isotopic balancing. It is unclear exactly what this means, but this could result in the minor isotopic differences between NPACC and NPACC-X. Despite these isotopic differences, the actual estimation of minor isotopic enrichment between NPACC and NPACC-X more closely match than their hydraulic estimations. Unfortunately, the estimation of minor isotopic separation is an undefined problem area with many different possible solutions, and NPACC-X only provides one possible solution to this area.

Ultimately, despite the differences in hydraulic and isotopic estimations between NPACC and NPACC-X, NPACC-X is still of value to the university as it provides a foundation for future work on uranium enrichment cascades. It utilizes the same underlying workflow as the original NPACC in the building of a uranium cascade but differs in its understanding of how these minor isotopes are enriched through the cascade. With more work and help, this model could repeat the successes of the original NPACC or even improve upon them with increased flexibility and availability.

Chapter 5

Future Work of NPACC-X

Despite the progress made by the university in the development of its own centrifuge cascade modeling tool, there remains much work to be done in order to bring this code into a more finalized position for future development and personnel training on the program. In short, this model still needs more work to be done in order to match the seminal work done under Dr. David Vermillion for his PhD dissertation on modernizing classical cascade analysis. This is because the university was not able to retain this initial version of the NPACC modeling tool, and the work must be recreated starting from an extremely early version of this code.

Firstly, the core benefit of the initial version of NPACC was its ability to model and predict the separation and enrichment of multi-component streams as they are passed through a centrifuge cascade. This capability was lost and has seen work in its redevelopment for this study. Unfortunately, although the new version of multi-component separation is included the rebuilt version of NPACC, its results do not match that of its predecessor and additional work must be done in order to achieve more reasonable estimates of multi-component enrichment. This has proved to be a difficult problem to solve as there is a lack of openly available information on the way that centrifuges separate multi-isotope streams resulting in an undefined problem space with many possible solutions. However, this author believes that with some more work and debugging, the rebuilt version of NPACC will be able to estimate multi-component separation values that more closely match the results of its predecessor than its current version.

Secondly, NPACC needs to be put into a more modernized programming language such as Python for ease of development and increased post-processing capabilities. Currently, this program's code base is fairly convoluted and as it grows, becomes increasingly harder to add in additional capabilities. Moving to Python would allow developers to reformat the underlying computational processes in a more flexible format while also improving on clarity of the variables, functions, and methods used for cascade modeling. Adding in additional enrichment technology parameters or increasing the flexibility of the program for non-ideal cascade designs would be much easier with a program built in Python. Additionally, Python is an extremely flexible language with a host of post-processing libraries that can improve the ability to graph and interpret the simulated data from the modeling program. Moving this code to Python would also allow for its use on classified systems as Matlab is currently unavailable in controlled areas due to its need for an internet connection while also circumventing the need for a costly Matlab license. Ultimately, a move to Python is necessary for the future development of this previously unobtained modeling tool.

5.1 Multi-Component Separation

Because the multi-component balancing in its current form does not agree with the original data produced in Dr. Vermillion's dissertation, more work would be needed to accurately analyze and predict the separation of multi-component streams through enrichment cascades. Although both Dr. Vermillion's dissertation and this study produce data that cannot be verified or validated due to the nature of the machines being studied, this does not mean that the data produced from this model is more accurate than its predecessor. In large scale cascades that mimic ideal cascades, there is a high level of agreement between the findings of MSTAR's multi-component separation and that of Dr. Vermillion's original NPACC. This is because in large-ideal cascades many of the assumptions about cascade analysis founded in gaseous diffusion hold true as there is minimal mixing and shaping losses. It is only when MSTAR and the original NPACC are used on unideal-small cascades where the difference in multi-component separation becomes apparent. It is in these small cascades where the original NPACC is believed to better predict minor isotopic separation due to

its calculation of mixing losses, shaping losses, and how the depletion of heavy isotopes affects the performance of individual machines. This leads to the belief that NPACC, in its original form, has set the "goalposts" for results of minor isotopic separation through unideal cascades.

Currently, NPACC-X, the form of NPACC derived in this study, does not greatly agree with the original findings of MSTAR or NPACC for both large-ideal and small-unideal cascades. In large-ideal cascades, NPACC and NPACC-X have a greater degree of agreement; however, hydraulic performances of the cascade are still underestimated along with small deviations of the multi-component enrichment. This is believed to be due to the way that minor isotopic cuts, separation factors, and atomic weight percentages are calculated on a stage-by-stage basis. Unfortunately, this problem is hard to find a solution for as the problem space is undefined due to the lack of openly available information surrounding multi-component separation through gas centrifuges, or any enrichment technology for that matter. Many forms of calculating separation factors, cut, and enrichments have been covered have been covered in the methodology section, but that still leaves the question of where to investigate next. This section will cover what the next possible path could be followed to arrive at proper multi-component separation through the enrichment cascade.

Although, the multi-component enrichment of NPACC-X is close to that of its predecessor, there still remains many possibilities for improving its performance in relation to multi-component separation. Currently, the isotopic separation factors of minor isotopes in large, ideal cascades is much higher for NPACC-X as compared to the original NPACC. Because these ideal cascades should have constant separation factors due to a lack of mixing or shaping losses, the difference between the separation factors of minor isotopes will probably lie somewhere in the development of the centrifuge performance maps. If the performance maps between NPACC and NPACC-X are yielding different base α_{mk} then this will result in a change in both the height and width of the cascade. This is due to the subsequent change in cut across all stages due to the different α values. The next steps in understanding multi-component separation should be in the area of re-verifying these performance maps and optimal feed rates for each enrichment machine.

5.2 Moving code base to Python

Because the move to necessary for the future development of this code, understanding how this move could be performed is important for this study. This will involve the explanation of the underlying data storage mechanisms for the cascade's physical parameters along with the overall program algorithm for how this data is transformed as a cascade solution for a given desired end use.

Firstly, it is important to understand what parameters would be of use for this port to Python and how they would be stored in a Python-based NPACC-X. The proposed solution would be to create individual stage objects corresponding to all necessary parameters associated with a group of separation machines. Initially, this would correspond to a series of objects stored on a stage-by-stage basis that each contain parameters needed for proper cascade analysis. These parameters would be the same as found in the methodology section. This would mean each object would contain nine (9) base parameters plus $3 * i$ isotopic parameters. Additionally, more parameters could be flexibly added to increase unideal cascade analysis such as the existence of side withdrawal or feed rates. Transferring these stage parameters would be beneficial for understanding how the underlying code works for future programmers as renaming stagewise variables would allow for increased comprehension of the physical parameters in question. In other words, something like stage (n)'s feed rate would look like E(2,n,1) whereas in python this would be self.stagenumber(n).feedRate. This is clearly more understandable than the former method of stagewise variable storage. Additionally, this method for storing stagewise parameters would allow for a dynamic storage of different isotopic feed vectors. For example, in the current version of NPACC-X, each space in the data storage matrix is hard coded to a minor isotopic enrichment value. Therefore, it has been hardcoded to only handle a possible isotopic vector of [U232, U233, U234, U235, U236, U238] and its corresponding isotopic mass. If a potentially new isotopic vector were to be fed into the existing version of NPACC-X that contained more or differently weighted isotopes than this uranium vector, then this version of NPACC-X would not be able to handle that isotopic stream. However, if the minor isotopic data storage were dynamically built, one could theoretically feed the cascade code with any number of isotopes with varying isotopic

masses. This would result in all the minor isotopic values being dynamically stored in a clean data structure that when called would look like self.stagenumber(n).isotope(i).alpha which would correspond to isotope (i)'s separation factor (alpha) at stage (n).

Next, it would be beneficial to take the pseudo-simulated annealing cascade routine and replace it with an actual simulated annealing routine that leverages an overall cascade performance metric and stochastic variation of cascade shape that dynamically changes as the optimization routine reaches a "most optimal solution." The former pseudo-simulated annealing routine simply checks to see whether the cascade is reaching the desired enrichment and product rate and will vary the overall feed of the cascade based upon overall cascade cut in order to reach the optimal feed rate while still maintaining enrichments necessary for the desired end use of the cascade. This means that the current optimization routine is not based upon a scientific simulated annealing routine that gradually decreases stochastic variation of variables in question until a most optimal result is found, but rather, this current version of the optimization routine only varies one component of cascade shape, the feed, and the final cascade solution is simply based upon whether the cascade with a given height and width meets the product throughput and enrichment levels needed for a desired end use.

In order to make this code more flexible, it would be beneficial to incorporate a real simulated annealing routine in which the cascade scoring is based upon how closely a cascade configuration reaches it desired end use on the basis of enrichment, throughput, and minimizing internal hydraulic reflux. This would mean that the cascade in question would be the most economical cascade configuration, by minimizing the number of machines necessary, for a given product enrichment and throughput. Additionally, this simulated annealing routine would allow for the varying of additional cascade parameters that would be included in future iterations of NPACC. For example, with the additional of a side withdrawal or feed parameter, NPACC could vary the potential re-piping combinations to determine if an abnormal cascade configuration would best meet a cascade's operating specifications. With the incorporation of this type of optimization routine, one could make estimations well outside the capabilities of normal cascade modeling codes. For example, a machine limiter could be incorporated into this optimization routine that would result in the code finding the most optimal cascade for a desired end use while still maintaining that the overall

cascade is limited in total number of machines. This would be useful for analyzing the proliferation potential of abnormal cascade operating conditions. This flexibility in cascade analysis would be unparalleled as it would allow for the analysis of an unideal cascade whose shape is being leveraged to reach a desired product end use. However, this feat would not be trivial as quantifying how "useful" a cascade shape is would be difficult while utilizing a single cascade "score." This is because this singular score would need to incorporate how well the cascade shape met the product enrichment and throughput while simultaneously quantifying how well the cascade shape minimized hydraulic reflux. In the end, it would still be beneficial to incorporate a real-life optimization routine, but more research would need to be done to develop an accurate cascade scoring method.

As for the overall cascade building routine, it would mostly remain the same between Matlab and Python as the overall algorithm is soundly based on the underlying science behind centrifuge performance as the code attempts to mimic a transient flow of product starting from the feed stage and working up/down to the heads and tails of the cascade. This means that the overall algorithm used in Python would be greatly similar to that of the one discussed previously in Chapter 3. The main difference in terms of the cascade building methodology between NPACC-X in Matlab and its potential future Python counterpart would be to the simulated annealing routine placed around the entire cascade building method. Hopefully, the changes to the both the cascade stage parameters and optimization routine in Python would result in a cascade code that is cleaner and easier to use than its Matlab predecessor.

There are still additional areas that could be further investigated to improve the overall flexibility and performance of this modeling program. For example, the implementation of a realistic transient analysis of multi-component separation would allow for the understanding of the proliferation potential of a cascade as it is first brought online. This is due to the varying effects that machine feed rate has on both the overall work done by each centrifuge machine and its corresponding separation factor. In other words, as an enrichment cascade is first brought online, its product throughput will be below that of its steady state operational counterpart, but the product enrichment would be much higher. As the machine feed rate is under-ideal during startup, the separation factor will increase across the entire

cascade resulting in a product that is above declared enrichment. A better understanding of transient multi-component separation would allow for nonproliferation analysts to determine the expected product enrichment levels at a given time during startup of the cascade. Additionally, this capability would allow for a better understanding of how the replacement of the centrifuge machines affects the overall isotopic vectors across each stage of the cascade. If a stage needs to have half of its machines removed and replaced, the GCEP will not shut down the entire cascade, but rather, only the machines in question. This will result in an abnormal cascade shape, even temporarily, which will have a rippling effect on the internal hydraulics and component separation throughout this cascade.

Further work could be done in the area of asymmetric separation. Currently, in both Dr. Vermillion's NPACC and this version, NPACC-X, it is assumed that each machine separates and depletes an isotopic vector equally at a given stage. In other words, the heads separation factor (β) and the tails separation factor (γ) are equal where $\alpha = \beta * \gamma$. In the current versions of NPACC, the heads and tails separation factors are considered equal so that both separation factors are calculated as $\sqrt{\alpha}$. In Python, an asymmetric separation factor would easier to incorporate as each stages heads and tails separation factor are stored dynamically on a stagewise basis for each isotopic constituent. Although this could be done in the existing codebase in Matlab, it would be much more difficult as it would require the reestablishment of fundamental stage parameters and their corresponding hundreds of lines of code that use this hard-coded separation factor variable. This asymmetric separation is closer to reality and would provide a level of resolution previously unobtained by open-source academia, and its incorporation into a Python based NPACC-X would be rather trivial compared to its current Matlab form.

Lastly, the future implementation of NPACC-X into Python would allow for the development of additional modules that use the information provided by the code to take empirical measurements of a cascade and compare them to the model's predictions. In other words, the model would predict a certain stage's physical parameters such as atomic weight percentage of a minor isotope and use this data to inform an empirical data measurement technique such as mass spectrometer wipes. Similarly, this model could incorporate a module that takes data from flow rate meters placed on specific stages of a centrifuge cascade which

would verify that a stage is producing or being fed the expected amount of feedstock for that position in the cascade. NPACC-X would be great for this as its previous counterpart under Dr. Vermillion was suspected to be much more accurate at estimating hydraulic reflux and incorporating mixing and shaping losses as compared to its predecessors.

Ultimately, this model still needs a lot of work to leverage the full computational capabilities available to the university in order to make a modernized, simplified, cascade modeling code. Despite its current flaws, NPACC-X provides a robust foundation that can be further refined to bring the university a one-of-a-kind enrichment cascade modeling program. Fixing the multi-component separation and hydraulic reflux should be the top priority of the future work on this model. Then, moving this code to Python for increased flexibility and ease of development would be the next step followed by the incorporation of more advanced cascade dynamics such as transient analysis or asymmetric separation.

Chapter 6

Conclusions

Because the establishment of uranium enrichment facilities is integral to the front-end of a peaceful NFC, they cannot be universally restricted across the globe. This means that it is up to the international nonproliferation community to best figure out how to safeguard these enrichment facilities while ensuring that they can produce fuel for peaceful nuclear power production. And as the technology behind gas centrifuge enrichment is gradually dispersed across the globe, it is imperative that the nonproliferation community continues to improve their characterization techniques of these dual-use technologies. Although NPACC-X does not give spatial parameters of modeled cascades similar to that of NPACC, it still provides the information necessary to better understand the proliferation risk of existing declared GCEPs. The basic information provided by NPACC-X, such as number of machines in a cascade and number of machines per stage, can still be used to estimate the spatial footprint of over-the-horizon declared GCEPs and clandestinely established GCEPs given an understanding of pilot-plant centrifuge spacing.

The original NPACC methodology developed by Dr. Vermillion has been shown to provide higher levels of resolution when dealing with the cascade's internal physical parameters using the newly developed "cascade dynamics" [16]. However, because this previously built codebase was lost on the university, it was imperative to rebuild the cascade code as best as possible. NPACC-X serves as a foundation for the rebuilding of this cascade code with respect to minor isotopic separation, the minimization of a priori knowledge, and

the modeling of non-ideal centrifuge cascades. Because both code bases cannot be verified or validated to existing data, this newly developed NPACC-X was benchmarked to the original NPACC and was found to be in close agreement with the minor isotopic separation processes, but still was left lacking in the proper estimation of hydraulic reflux inside the cascade.

Both NPACC and NPACC-X are valuable tools to future nonproliferation analysts as they both rely on a minimal amount of a priori knowledge of the cascade in question. In both codebases, the user simply needs to know the desired end use of the cascade, the feedstock assay vector, and the depletion rate of the cascade, which can be derived from the economic costs of uranium ore. Realistically, this leaves the user with only having to know what the cascade is declared to produce in terms of enrichment and material throughput and the feedstock of this cascade because the depletion rate of the UF_6 can be calculated from economic conditions of the uranium ore. As the ore becomes more expensive, GCEP operators are motivated to deplete the uranium further as the price of the U^{235} in the tails assay of the cascade becomes more valuable. Ultimately, NPACC-X provides a previously unobtained cascade modeling tool to The University of Tennessee and can be of great use in the space of open-source cascade modeling. Although initially designed for centrifuge cascades, NPACC-X is flexible enough to handle different types of enrichment technology so long as they adhere to the normal first-order principles of elemental separation. In other words, so long as the separation technology contains variables associated with centrifuge performance maps such as separation factor, cut, or separative work, NPACC-X can be modified to handle these different enrichment technologies. NPACC-X stands as the first cascade modeling tool that incorporates cascade dynamics that will be available to the university. This is the first tool of its kind to be held by the university that can more accurately assess non-ideal centrifuge cascades and multi-component separation.

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Appendices

A Summary of Equations

Isotopic separation factor:

$$\alpha_{jk} = \alpha_0^{\frac{MW_{heavy}-MW_j}{MW_{heavy}-MW_{light}}} \tag{1}$$

How much a two component system gets enriched by a single machine at stage (n):

$$X_{j_{n+1}} = X_{j_n} * \sqrt{\alpha_{jk}} \tag{2}$$

How much a two component system gets depleted by a single machine at stage (n):

$$X_{j_{n-1}} = X_{j_n} * \frac{1}{\sqrt{\alpha_{jk_n}}} \tag{3}$$

Overall Stage Cut:

$$\theta = \frac{\dot{P}}{\dot{F}} \tag{4}$$

Separative Capacity:

$$\Delta U(SWU) = \dot{P}{V_2}^y + \dot{T}{V_2}^z + \dot{F}{V_2}^x \tag{5}$$

Where:

$${V_2}^n = (2n-1)\ln(\frac{n}{1-n}) \tag{6}$$

A.1 Stagewise Calculations

Individual Component Enrichment level at stage (n):

$$X_{j_n} = \frac{\dot{P}_{n-1} * X_{j_{n-1}} * \alpha_{mk}^{\frac{MW_{heavy}-MW_j}{MW_{heavy}-MW_{light}}} + \dot{T}_{n+1} * \frac{X_{j_{n+1}}}{\alpha_{mk}^{\frac{MW_{heavy}-MW_j}{MW_{heavy}-MW_{light}}}}}{\dot{P}_{n-1} + \dot{T}_{n+1}} \tag{7}$$

Stage feed rate at stage (n):

$$\dot{F}_n = \dot{P}_{n-1} + \dot{T}_{n+1} \tag{8}$$

Optimal number of machines at stage (n):

$$Machines = \frac{\dot{F}_n}{L_{opt}} \tag{9}$$

Where L_{opt} is the optimal feed rate of the machine in question and then the number of machines is rounded down to the next integer value.

Average Machine Feed Rate at stage (n):

$$FR_{machine} = \frac{\dot{F}}{Machines} \tag{10}$$

Overall stage cut at stage (n):

$$\theta_{mk} = \frac{(1 + \sqrt{\alpha_{mk}^{\frac{MW_{heavy} - MW_j}{MW_{heavy} - MW_{light}}}} - 1) * X_{235n}}{1 + \sqrt{\alpha_{mk}^{\frac{MW_{heavy} - MW_{235}}{MW_{heavy} - MW_{light}}}}} \tag{11}$$

Stage product rate at stage (n):

$$\dot{P} = \dot{F}_n * \theta_{mkn} \tag{12}$$

Stage tails rate at stage (n):

$$\dot{P} = \dot{F}_n * \frac{1}{\theta_{mkn}} \tag{13}$$

B NPACC vs. NPACC-X Output Comparisons

Cascade Shape and profile	Ideal Black Box	NPACC_2 David's Version	1987 MSTAR	NPACC_X David's Version	NPACC_X Patrick's Version	Difference %
Total Stages	23	23	23	23	23	0
Enriching Stages	14	14	14	14	14	0
Stripping Stages	9	9	9	9	9	0
Total Number of Machines	4947	5161	366	5384	3483	-35.30
Cascade Cut	.1102	.1139	.1137	.1090	.1149	-5.41
Optimal Feedrate (kgU/yr)	187,634.963	181,210.07	181,536.36	189,338.72	180,251.98	-4.79
Product Rate (kgU/yr)	20,641.95	20,635.31	50,641.95	20,638.19	20,719.13	0.39
Tails Rate (kgU/yr)	166,707.67	160,574.76	160,894.41	168,700.53	160,240.5	-5.01
Total Separative work (SWU/yr)	264,855.57	278,100.89	19,596.64	290,110.17	187,667.9	-35.31

Figure B.1: Output comparisons between NPACC and NPACC-X for Rome cascade for full scale VVER-1000. Data from first 4 columns taken from [16]

.

Product

Isotope	MSTAR Product	NPACC David	NPACC-X	% Diff
U238	0.94847	0.94837	0.9485	0.014
U235	0.05107	0.05088	0.0507	-0.354
U234	0.00045	0.00075	0.0075	0.000

Tails

Isotope	MSTAR Product	NPACC David	NPACC-X	% Diff
U238	0.99818	0.99824	0.9946	-0.36
U235	0.00181	0.00175	0.0015	-14.28
U234	0.00001	0.00001	0.0000069	-31.0

Figure B.2: Output comparisons between NPACC and NPACC-X for Rome cascade for full scale VVER-1000. Data from first 4 columns taken from [16]

.

Cascade Shape and profile	Ideal Black Box	NPACC_2 David's Version	1987 MSTAR	NPACC_X David's Version	NPACC_X Patrick's Version	Difference %
Total Stages	25	25	26	26	27	3.85
Enriching Stages	14	14	13	13	14	7.69
Stripping Stages	11	11	13	13	13	0
Total Number of Machines	3,489,902	4,063,233	239,705	4,013,566	3,178,201	20.81
Cascade Cut	.1605	.1508	.1815	.1727	.1506	12.79
Optimal Feedrate (kgU/yr)	11,090,343.57	11,801,131.74	9,805,765.05	10,308,219.98	11,814,139.76	14.61
Product Rate (kgU/yr)	1,779,776	1,779,781.22	1,779,776.1	1,779,777.6	1,779,784.86	.00004
Tails Rate (kgU/yr)	9,310,567.47	10,021,350.18	8,025,988.97	8,528,442.05	10,034,402.59	17.65
Total Separative work (SWU/yr)	15,390,469	17,684,231	1,057,099	17,468,068	13,832,000	20.81

Figure B.3: Output comparisons between NPACC and NPACC-X for Iguacu cascade for full 65 PWR fleet. Data from first 4 columns taken from [16]

.

Isotope	MSTAR Product	NPACC David	NPACC-X	% Diff
U238	0.93634	0.93375	0.9343	.0059
U235	0.04808	0.05437	0.0512	5.830
U234	0.00096	0.00166	0.0018	8.434
U236	0.01462	0.01022	0.0127	24.25
U232	8.41E-09	3.99E-08	4.8874E-08	22.50

Figure B.4: Output isotopic comparisons between NPACC and NPACC-X for Iguacu cascade with RepU feed for HFIR. Data from first 4 columns taken from [16]

.

Cascade Shape and profile	Ideal Black Box	NPACC_2 David's Version	1987 MSTAR	NPACC_X David's Version	NPACC_X Patrick's Version	Difference %
Total Stages	48	49	54	54	52	-3.73
Enriching Stages	37	38	41	41	39	-4.87
Stripping Stages	11	11	13	13	13	0
Total Number of Machines	7200	3317	379	12421	2817	-77.3
Cascade Cut	0.0081	0.0177	0.0156	0.00056	0.01575	-27.12
Optimal Feedrate (kgU/yr)	14921.25	6826.3	7748.35	21776.64	7644.5	-64.89
Product Rate (kgU/yr)	121.14	121.02	121.14	121.09	120.42	-.553
Tails Rate (kgU/yr)	14800.11	6704.95	7627.21	21655.22	7481.8	-65.45
Total Separative work (SWU/yr)	31750.22	14432.87	1671.39	54056.85	12254.77	-77.33

Figure B.5: Output comparisons between NPACC and NPACC-X for Iguacu cascade with RepU feed for HFIR. Data from first 4 columns taken from [16]

.

Isotope	MSTAR Product	NPACC David Product	NPACC-X Product	% Diff
U238	0.31253	0.00000	0.0000 – 0.0346	0
U235	0.54961	0.91110	0.8117 - 0.9549	0
U234	0.01142	0.08603	0.0779 – 0.1002	0
U236	0.12645	0.00285	0.0758 – 0.0815	2559.6
U232	1.00E-07	1.97E-05	1.4921E-05 – 2.2966E-05	0

Isotope	MSTAR Tails	NPACC David Tails	NPACC-X Tails	% Diff
U238	0.99594	0.99729	0.9897	-0.761
U235	0.00190	0.00146	0.0014	-4.11
U234	0.00001	0.00001	0.000015	50.0
U236	0.00216	0.00124	0.0012	-3.22
U232	9.15E-12	3.44E-11	3.8064E-11	10.6

Figure B.6: Output comparisons between NPACC and NPACC-X for Iguacu cascade with RepU feed for HFIR. Data from first 4 columns taken from [16]

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Vita

Patrick Williams grew up in Oak Ridge, Tennessee and subsequently has had his life shaped by the discovery of fission and the development of the Manhattan project. The nuclear industry seemed very commonplace throughout his childhoood and it would not be until his senior year of high school that he began to look at it in a different light. Nuclear power changed from a commonplace industry in his hometown to a potentially world changing industry that could be poised to solve clean energy production demands in developing countries after he watched a video on advanced generation III and IV reactors. This motivated him to attend the University of Tennessee, Knoxville and pursue a degree in nuclear engineering as a means to tackle one of the largest problems facing humanity in the coming century. However, after completing a co-op rotation with Southern Nuclear Operating Company at Plant Farley, Alabama, he switched his focus from wanting to just participate in nuclear energy production to actively solving the coming problems of the nuclear industry. After returning to UT from Dothan, Alabama, he began undergraduate research helping to develop a new centrifuge cascade model with Dr. David Vermillion for his PhD dissertation in hopes of better understanding uranium enrichment centrifuge cascades. His programming background allowed for him to help Dr. Vermillion develop a new model based on "cascade dynamics" that proved to be a large step forward in modeling the internal physical characteristics of a centrifuge cascade. This success motivated him to attend graduate school at The University of Tennessee where he continued working on centrifuge modeling programs for both Oak Ridge National Lab and UT. During his time in graduate school, he has worked to develop more advanced assay measurement techniques through the use of femtosecond laser induced breakdown spectroscopy (LIBS) at UT. Additionally, he spent his summers in graduate school in the Computational Fluid Dyanmics (CFD) group

at ORNL and the Computational Physics Division at Los Alamos National Lab. At ORNL he utilized his computer science knowledge to develop an open source CFD program that utilized Sandia National Lab's CUBIT geometry mesh tool to generate complex geometry meshes for OpenFoam. At LANL, he helped computer scientists write python bindings for a C++ library that interacts with ACE data tables to be used for charged particle transport. As he finishes his Master's Degree, he hopes to continue work in the nonproliferation sector with the goals of achieving nuclear disarmament while maintaining peaceful nuclear power production. Currently, he lives in Knoxville, Tennessee with his family and two cats and is looking for some new problem he can solve to better protect the world.