

May 1, 2021

Dr. Robert Counce
CBE 488
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Dear Dr. Counce:

We are submitting the attached report entitled Process Design and Economic Analysis of Thorium Dioxide and Rare Earth Elements Extraction from Monazite Clay.

This report examines the results of designing a process and estimating the capital and manufacturing costs for the overall process.

I hope you find this report satisfactory.

Sincerely,

Katherine Glass, Connor High, Jason Pan, Ei Jenkins, and Niall Terry

Honors Design in Green Engineering
University of Tennessee
Knoxville, Tennessee

Enclosure: Final Report

Process Design and Economic Analysis of Thorium Dioxide and Rare Earth Elements Extraction from Monazite Clay

CBE 488: Honors Design in Green Engineering

Submitted:
May 1, 2021

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Acknowledgements

Dr. Counce, University of Tennessee

Patrick Zhang, Florida Institute of Industrial and Phosphate Research in Bartow, Florida

The Electric Power Research Institute (ERPI)

1.0 Introduction

This report will detail the process of isolating thorium dioxide from monazite ore as well as a capital and manufacturing cost analysis of implementing the process. In order to accurately describe the process of separating thorium dioxide from monazite ore flow sheets, material balances, and simulations using software are used. The capital and manufacturing costs will then be estimated using the ChE index value of 595.5 for 2021.

The idea of using thorium as an alternative to uranium has been a subject of interest that has been present for quite some time as thorium has several qualities that make it a better option. There are several reasons this can be attributed to; first and foremost, thorium is more abundant in nature as compared to uranium. In addition, thorium fuels can breed fissile uranium-233 to be used in various kinds of nuclear reactors. Molten salt reactors are well suited to thorium fuel, as normal fuel fabrication is avoided. Considering these advantages, the process of using thorium is one that remains desirable for investigation.

The primary design objective of this study is to investigate the use of thorium in a once-through fuel cycle for future nuclear reactors. This includes the design and analysis of a process to produce reasonably pure thorium dioxide (ThO_2) and rare earth oxides as a bi-product from monazite ore using a rotary kiln, taking into account the effects of impurities. An optimization analysis of the process is conducted while considering human health, the environment, and economics.

The feed rate desired for this process is 1000 kg/hr of monazite. This monazite ore is to produce reasonably pure ThO_2 as a product along with rare earth oxides as a bi-product. The bi-product stream includes trace amounts of: Uranium (in PO_4 form), silicon (as SiO_2), calcium (as CaF_2) and iron as (FePO_3).

With the desired objectives, there are a few restrictions that need to be considered to keep the process safe. The desired reaction is completed at low temperature $< 300\text{ C}$ in order to keep the process less expensive and safer to operate. The only process steps that exceed this temperature are the production of rare earth oxides using a calciner or rotary kiln. Specific to this process, it is important to protect the workers, community, and environment from radon. Personal protective equipment (PPE) should be issued to all workers due to possible exposure to radon and/or other radioactive materials involved in the process. When working with radioactive materials, it is vital to “house in” any radiation that may pose a health hazard to workers. Concrete, lead, or other radioactive barriers should be involved with the construction of unit processes housing radioactive materials. For the environment, proper disposal and/or repurposing of by products of thorium dioxide purification must follow the national Environmental Protection Agency (EPA) and state guidelines to ensure the environmental impact is nullified and that the plant receives no fines or lawsuits from improper handling of waste materials.

To efficiently achieve project goals, as well as acknowledge and conform to project restrictions, OLI Flowsheet software is implemented to simulate and optimize the processes utilized to separate and isolate the thorium dioxide and rare earth elements (REEs) from the monazite ore. The monazite ore is reacted with concentrated sulfuric acid creating multiple phases and dissolved species. The species are separated via several more reactions, evaporations, and solid-liquid separations.

Contributions to this study were provided by Patrick Zhang of Florida Institute of Industrial and Phosphate Research in Bartow, Florida, the Electric Power Research Institute (EPRI), and the University of Tennessee, Knoxville (UTK).

2.0 Synthesis Information for Processes

2.1 Overall Preliminary Process Design

The preliminary design for the extraction of thorium from monazite ore starts by feeding monazite ore, water and sulfuric acid into a rotary kiln to react. After the reaction occurs, the solution is cooled down via a heat exchanger so that the thorium sulfate precipitates from the solution as a solid. The thorium sulfate solids are then extracted via a separator. The remaining metal sulfates are then transferred into a waste stream to be neutralized. Once separated, the thorium is fed to another reactor along with sodium hydroxide in order to convert the thorium sulfide into thorium oxide. The waste liquid is then fed to a mixer to neutralize the basic waste, while the thorium is taken as a pure product.

The preliminary design for the extraction of thorium from monazite ore was improved upon to further refine other metals from monazite ore. Monazite contains significant amounts of Neodymium, Lanthanum, and Cerium among other metals that could be extracted and sold as byproducts. This further extraction will decrease the amount of waste created from the process as well as provide more profits for the plant.

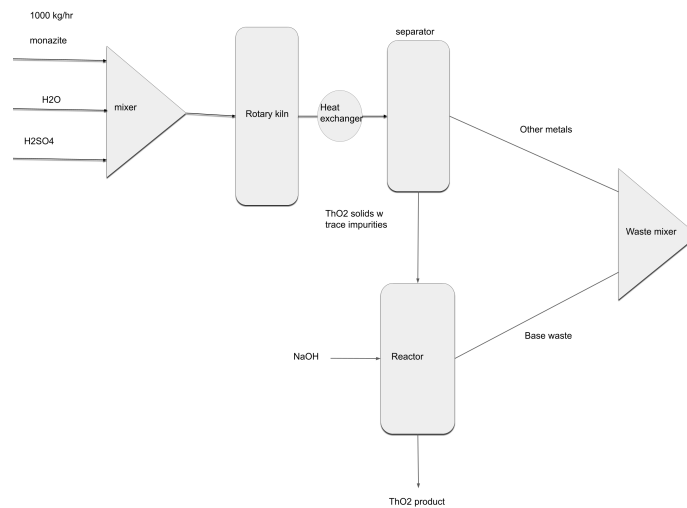


Figure 1. Initial process design.

2.1.1 Process Constraints

Our design aims to produce >99% pure thorium dioxide, as well as rare earth oxides as a valuable byproduct, from monazite ore. The feed rate of monazite is to be 1000 kg/hr, and the conversion of monazite ore to sulfates must be done using a rotary kiln. In order for this process to be successfully competitive, the products must be more economically viable than the raw materials. Legislation protecting worker and community health as well as the environment (in particular radon hazards) are to be followed and exceeded in the design of this process.

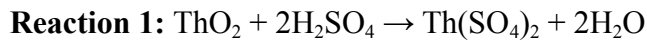
This process design will be conducted utilizing OLI software. OLI software predicts properties of multi-component, multi-phase systems using models. These models can be reasonable, however, they cannot predict the actual behavior of systems. There is always a level of uncertainty when using predictive models. Our analysis is bounded by the constraints of the models used in OLI. For example, OLI accounts for thermodynamics but not kinetics. Physical experimentations are required to fully understand the processing conditions. In addition, OLI does not account for particle size.

Equipment design must also conform to specific constraints. Some reactors need to be capable of handling high heat and high pressures (up to 300 C and 50 atm). Other reactors need to be made from materials that can resist corrosion from acids such as sulfuric acid and hydrochloric acid.

In accordance with worker and environmental safety standards, waste streams must be acceptable pH and composition when exiting the plant for wastewater treatment. In addition, there are issues of nuclear criticality when processing radioactive materials such as thorium and uranium that require special analyses and design.

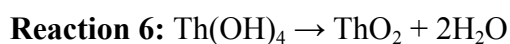
2.2 Final Process Chemistry

The separation processes begin with the initial feed of raw monazite ore being processed in a rotary kiln with sulfuric acid. Following the process outlined in Demol, et. al 2018, the monazite ore is reacted with excess sulfuric acid at 250°C for 2 hours. Here, the following reactions occur between the monazite ore and sulfuric acid solution allowing for the REE's and thorium to be leached from the raw ore:



Leaving the rotary kiln, a slurry of water, phosphoric acid, and thorium and REE sulfates (S-1) are contacted with a stream of additional phosphoric acid in a reactor (R-1). In this reactor, the pressure is increased to 15 atm and the temperature drops to 200°C. This allows for the thorium sulfate to precipitate from solution. As a result of the addition of phosphoric acid, the previous reactions 2-4 have their equilibrium reversed returning the REE sulfates back to their phosphate forms.

The resulting slurry is delivered to Filter-1 where the solid thorium sulfate (S-4) is separated from the other components (S-5). The thorium sulfate stream (S-4) is then contacted with a stream of sodium hydroxide and water (S-6) in Reactor-2 where the temperature and pressure are reduced to 103.8 °C and 1 atm respectively. The two following reactions occur where the thorium sulfate is converted to thorium hydroxide and successively thorium oxide under these conditions:



The products of these reactions (S-7) are passed through a heat exchanger where the temperature and pressure are altered to 50°C and 2 atm. The resulting stream (S-10) is sent to a mixer (Mix-1) where it is contacted with an additional stream of water (S-13). This water stream is necessary to dissolve all other compounds in the mixed stream except for thorium oxide. From the mixer, stream 14 (S-14) is delivered to Filter-2 where the solid thorium oxide (S-8) is separated from the aqueous waste stream (S-9). The solid thorium oxide is collected as the primary product of the process and the waste stream is sent to be neutralized.

The aqueous REE stream (S-5) leaving Filter-1 is delivered to an extractor where the phosphoric acid (S-11) is removed from the aqueous stream. This multistage separator, described in section 4.2.2, results in the phosphorus being removed from the solution pushing the equilibrium toward the products side of the following reactions as phosphoric acid is removed. As a result, the REE's return to their sulfate forms via Reactions 2-4 as they exit the phosphoric acid extractor in the aqueous stream.

The aqueous REE sulfate stream leaving the extractor (S-12) is sent to a reactor (R-3) where it is contacted with a stream of sulfuric acid and water (S-15). The temperature rises slightly to 206°C but the pressure is reduced to 5 atm from 15 atm. This further addition of sulfuric acid solution adds driving force to the conversion of the REE's to their sulfate forms while reducing the necessary pressure. The mixed stream (S-16) is delivered to Filter-3 where the lanthanum and cerium sulfates are separated from their neodymium counterpart. This is an important step with regard to neodymium isolation since neodymium seems to only precipitate within the same range of temperatures and pressures as lanthanum and cerium; therefore, all lanthanum and cerium must be removed in order to provide a pure neodymium oxide stream. The lanthanum and neodymium sulfate stream (S-17) is sent as waste to be neutralized. The neodymium stream (S-18) series of steps aimed at recovery of water and sulfuric acid. These steps are outlined below in Section 4.2.5. Leaving this section of the plant, the neodymium sulfate stream (S-20) enters a heat exchanger (Heat Exch-3)

where the temperature is dropped from 240°C to 30°C and the pressure is reduced from 10 atm to 3 atm. Due to this condition change, the neodymium sulfate adds eight hydrate molecules forming the precipitate neodymium sulfate octahydrate (S-24). This precipitate is separated from the other components in Filter-4 and exits in Stream-26 (S-26). The aqueous stream (S-25) is sent to waste to be neutralized.

The stream of neodymium sulfate octahydrate is contacted, in Reactor-4, with a stream of sodium hydroxide solution at 100°C and 10 atm. Under these conditions, OLI specifies that the following reaction occurs where neodymium is converted from the sulfate form to a hydroxide:



The resulting product stream (S-28) is sent to a mixer (Mix-2) where, as before with the thorium hydroxide, water (S-29) is added to dissolve the other compounds in the stream (S-28) leaving only neodymium hydroxide as a solid product (S-30). The solid neodymium hydroxide (S-32) is separated from the other aqueous components (S-31) in Filter-5 and is sent to a calciner where, under high heat (600°C), hydroxides are converted to oxides via the following reaction:



The waste streams from Filter-2, -3, -4 and separator-2 (S-9, -17, -25, -34) converge and are mixed together (Mix-3). The resultant stream (S-37) is sent to the neutralizer where a sodium hydroxide solution is added to raise the pH of the waste stream to acceptable levels. The base reacts mainly with the two REE sulfates removed earlier to form hydroxides at a neutral pH as shown in the following reactions:



2.2.1 Property Data

OLI Flowsheet provides much of the necessary thermodynamic and property data for the given components of the system. For property data not available in OLI, outside references are used. Data pertaining to thorium or uranium is found in “Thermophysical Properties of Thorium and Uranium Systems for Use in Reactor Safety Analysis.” by Fink, et al. Rare Earth oxide property data is found in “Thermochemistry of the Rare Earths. Part I. Rare Earth Oxides. Part II. Rare Earth Oxysulfides” by Gschneidner, et al. Finally, a method for determining the solubility of compounds, especially those close to this system, is found in “Rare-Earth Leaching from Florida Phosphate Rock in Wet-Process Phosphoric Acid Production” by Liang, Haijun, et al.

2.3 Literature Review

Monazite is a rare earth (RE) phosphate which, out of the 200 of the best known minerals containing REEs, contains the second most significant amounts of materials such as thorium and uranium [2]. Thorium, found as an associated metal in monazite, is an important source of nuclear energy and is more abundant than uranium. Due to its importance in energy production and natural availability, future research and development in nuclear energy may create a focus on the utilization of thorium [1].

To isolate thorium from the other REEs within monazite, monazite must be cracked through one of two methods; a basic process with a sodium hydroxide solution where thorium and uranium are separated as a hydroxide or an acidic process with sulfuric acid where a liquor of REEs, thorium and uranium are produced [2]. In most cases, the basic process using sodium hydroxide is used [3]. Through these processes very high purifications of thorium and uranium have been achieved with recoveries of 99.9% and 99.4% respectively. Average thorium content within monazite is found to be 5 - 10% in U.S. deposits [1].

Along with its motivating natural abundance, thorium dioxide captures large revenue generation based on assumed market prices. Thorium product is worth almost twice that of the uranium product, \$80/kg and \$45/kg respectively. In addition to these two important REE products, monazite also contains significant amounts of neodymium which, when separated from the other trace REEs, captures approximately 10% more revenue than thorium [2]. The process of producing thorium from monazite is not only influential for the utilization of a more abundant resource but also for its key role in driving the economic potential for the production process.

2.4 Basic Process Economics

In order to complete this study level design and analysis of the ThO₂ production process a cost analysis of thorium oxide recovery from monazite ore must be considered. The economical points considered for the process include the costs of raw materials, equipment and manufacturing costs, and the recovery of our major product thorium oxide and other profitable byproducts. Energy costs for the process are determined using electricity as the primary utility. The resulting cost and details are presented in Table 1 is the cost information for the products and raw materials [1].

Table I. Raw Materials, Products, and Energy Cost

Item	Cost
<i>Product</i>	<i>\$/kg</i>
ThO ₂	\$80.00
Nd ₂ O ₃	\$47.00
P ₂ O ₅	\$2.00
<i>Feed</i>	<i>\$/kg</i>
Monazite	\$1.00
H ₂ SO ₄	\$0.04
NaOH	\$0.03
H ₃ PO ₄	\$0.80

3.0 Method of Approach

3.1 Initial Flowsheet Design

In order to separate thorium dioxide from monazite ore, monazite is first ground into a fine powder and mixed with sulfuric acid. The solution is then reacted in a rotary kiln so that the metal oxides are reacted to form metal sulfates. Thorium sulfate then precipitates out of the solution by cooling and running through a settler. The rare earth byproducts are transferred to a neutralizer. The precipitated thorium is transferred to a reactor with sodium hydroxide to convert it back to thorium dioxide and is separated from the solution. The basic waste from this reactor is then sent to the neutralizer to neutralize rare earth metals. This simplified process served as our initial design and was improved upon substantially to create the final process.

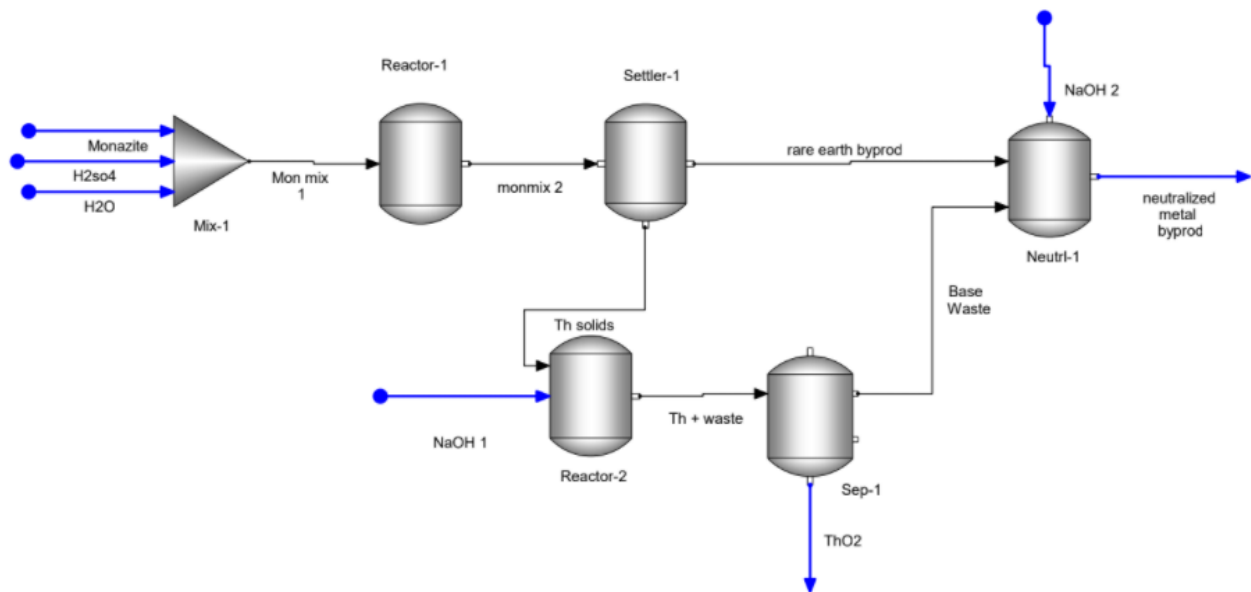


Figure 2. Simplified flowsheet design.

3.2 Sustainability, Environment, and Worker Safety

The use of thorium as a more sustainable alternative to uranium is a major reason in our execution of this project, first and foremost, thorium is more abundant in nature as compared to uranium. In addition, thorium fuels can breed fissile uranium-233 to be used in various kinds of nuclear reactors. Molten salt reactors are well suited to thorium fuel, as normal fuel fabrication is avoided. The need for an abundance of fuel is reduced through the use of thorium. Thus, their potential as a more sustainable method for nuclear energy extraction demands a viable method for thorium oxide extraction. Regarding environmental safety, the most concerning aspect of this design will involve the proper handling of the wastewater as well as the waste streams. The raw materials that are used in this study are potentially harmful to the environment and, thus will be handled according to government guidelines. Regarding the process of thorium oxide extraction from monazite ore, there is a significant environmental and worker safety risk associated with the radioactivity of thorium. In addition, the rare earth elements are toxic to humans, and the strong acids and bases utilized throughout the process can harm workers if proper precautions are not taken. A comprehensive outline of the hazardous raw materials is presented in section 4.3. We refer to guidelines laid out by OSHA, CWA, CAA, EPCRA, and Nuclear Criticality analysis for both environmental and worker safety.

3.3 Product Quality

Of any design considerations, product quality is among the most important. To achieve maximized profit (of that of the assumed market of the RE metals in table 1.) and to ensure the purity of thorium for utilization in energy production, the quality of the product streams must be ensured in our design. For the thorium dioxide product stream, a purity of >99% is a set goal to achieve. This will be achieved by allowing thorium to precipitate along with SiO₂ as a byproduct, dissolving the SiO₂ in a 5.35 M NaOH solution and filtering out the thorium product stream. While the major focus of this process is to achieve >99% thorium, the

byproduct stream will contain multiple valuable RE metals and should also be purified as to maximize process profit. Neodymium, the second most valuable of all the present RE metals, has the largest mass percentage and if purified can reap a larger value than that of purified thorium. This purification process will also utilize NaOH to dissolve contaminant phosphates that will then be filtered from the neodymium product stream.

3.4 Project Outline

The first draft of this project is to be submitted by April 15, 2021. After making corrections based on the reviewer's comments, the final document will be submitted by April 28, 2021. The assignment list with expected completion dates is shown below as it currently stands on February 17, 2021.

Table II. Project outline.

CBE 488 GROUP 6 SENIOR DESIGN PROJECT					
TASK	START DATE	DUE DATE	% COMPLETE	NOTES	
Project Introduction	1/20/21	1/27/21	100%		
Synthesis	2/3/21	2/10/21	100%		
Method of Approach	2/15/21	2/17/21	100%		
Initiate Flowsheet (~15%)	2/15/21	2/17/21	100%		
Flowsheet 25% Complete	2/17/21	3/3/21	60%		
Flowsheet 50% Complete	3/3/21	3/10/21	30%		
Flowsheet 75% Complete	3/10/21	3/17/21	20%		
Flowsheet Complete (100%)	3/17/21	3/31/21	15%		
Capital Cost Estimates	2/24/21	3/17/21		Work on ~2 pieces of equipment per week	
Manufacturing Cost Estimates	2/24/21	3/17/21			
Economic Analysis	2/24/21	3/17/21			
Report Writing 50% Complete	2/24/21	3/17/21	40%		
First Draft of Report	3/17/21	4/1/21	20%	Revise pending comments	
Submit Final Report	4/1/21	4/28/21	15%		

4.0 Results

4.1 Optimization

To ensure the retention of optimal system performance, multiple conditions were set to make the thorium dioxide extraction process sustainable and efficient. Due to the very large flow rates present throughout the system, immense quantities of water were also flowed into the reactors and neutralizers. To reduce the cost of larger unit operations, as well as the cost of water, recycle flow streams are implemented at certain separators to remove excess water that would otherwise be unutilized as waste. These recycled water streams can then be directed back into the monazite feed mixer, neutralizers, reactors, and other locations throughout the plant. Certain separations performed in the system are optimized to produce the maximum recovery of excess water as possible, by increasing temperature and decreasing pressure within the separator. The neutralization of waste streams was vital for optimization of the overall extraction process, to ensure compliance with environmental regulations the pH of each waste stream was raised to the neutral pH of 7. Without this neutralization the plant could lose profit in the form of fines or extra cost of waste processing by 3rd parties.

4.2.1 Initial Processing of Monazite Ore by Rotary Kiln

Outside of OLI simulation capabilities is the pyroprocessing unit operation used for metal extraction, the rotary kiln. Outside calculations on costing and estimations on rotary kilns can be found in appendix C.7. 1000 kg/hr of monazite is flowed into the kiln along with H_2SO_4 where the metal phosphates present in the ore are reacted into metal sulfates and phosphoric acid at 250 °C for 2 hours. The output, a slurry of metal sulfates, is then mixed with water (The mixed stream shown as S-1, in figure 3.) and fed into a hydrolysis reactor where the first step of the system can be simulated.

4.2.2 Thorium Extraction

The monazite metal sulfate slurry (S-1), along with 5000 mol/hr of H_3PO_4 , is fed into a hydrolysis reactor (R-1) set to operate at 200 °C and 15 atm. The resulting reaction produces Cerium, Lanthanum, Neodymium in soluble phosphate forms, allowing for filtration and isolation of the precipitated thorium sulfate in from the rest of the rare earth elements (S-5) in Filter-1. Next, the isolated thorium sulfate stream (S-4) and a 19.2 M NaOH stream is fed into reactor 2 (R-2) at 100 °C and 1 atm, resulting (S-10) in the production of the target product Thorium dioxide (ThO_2). This reaction produced the byproduct Sodium sulfate which would be found in a solid product with ThO_2 if filtered, to combat this, 6000 mol/hr of water was introduced through a mixer (Mix-1) which hydrolyzed all Sodium sulfate present. The resulting stream is then filtered (Filter-2) producing pure ThO_2 in the solid stream (S-8). The aqueous waste stream is then sent to waste neutralization.

4.2.3 Phosphorus pentoxide Extraction (Phosphoric acid recovery)

Phosphorus pentoxide (P_2O_5) is present in large amounts in the aqueous stream (S-5) flowing out of filter-1 and can bring large amounts of profit if extracted. (Phosphoric acid breaks down into P_2O_5 and

(P_2O_5)₂ in water.) Due to OLI limitations, isolation of P_2O_5 by an extractor was found to be nearly impossible. Due to this, a component splitter was implemented to simulate a series of multi-stage extractors that could isolate the phosphoric acid constituents in the purity seen in S-11. Costing and condition estimates can be found in Appendix C.9.

4.2.4 Cerium/Lanthanum Extraction

Post phosphoric acid recovery, the rare earth element containing stream (S-12) is fed into reactor 3 (R-3) with a 13.4 M solution of H_2SO_4 . The reaction conditions were set to operate at 200 °C and 15 atm. The resulting reaction reacts Cerium, Lanthanum and Neodymium into their sulfate forms: $\text{Ce}_2(\text{SO}_4)_3$, $\text{La}_2(\text{SO}_4)_3$ and $\text{Nd}_2(\text{SO}_4)_3$ respectively (S-16). This stream is then fed into filter-3 where the precipitated cerium and lanthanum sulfates are removed by the solid stream (S-17) leaving $\text{Nd}_2(\text{SO}_4)_3$ in the aqueous stream. The cerium and lanthanum sulfates are then treated as waste and sent to neutralization due to the immense cost of treating them into their profitable oxide forms and minimal price they can be sold at. Further alteration of the cerium and lanthanum sulfate stream can be made if future financial motivation is developed.

4.2.5 Water Recycle Stream 1 & Sulfuric acid Recovery

The aqueous out-put stream (S-18) of filter-3 flows at 36,601 mol/hr consisting of 29,500 mol/hr of H_2O and 3600 mol/hr of unneeded sulfuric acid. To minimize water consumption and save material cost of larger unit operations, large amounts of H_2O and H_2SO_4 are separated from the $\text{Nd}_2(\text{SO}_4)_3$ containing stream. For the largest water vapor production, the pressure and temperature of S-18 must be raised. From 207 °C and 5 atm, pump-1 and heat exchanger-2 raised the conditions entering the separator (Sep-1) to 240 °C and 10 atm. The separator achieved 17,028 mol/hr captured from the vapor outlet (S-19) and 8970.86 mol/hr of

H₂SO₄ recovered through the organic outlet (S-21), a 99.994% recovery. The rare earth containing aqueous output stream (S-20) then flows at 3988.19 mol/hr, an 88.34% reduction.

4.2.6 Neodymium Extraction

S-20 is fed through heat exchanger-3 to decrease its temperature to 30 °C. Lowering the stream temperature allows the neodymium sulfate to precipitate in a hydrate form. The stream (S-24) is then fed into filter-4 separating the neodymium sulfate in the solid stream (S-26) from the aqueous waste outlet. Next, the neodymium sulfate stream is fed into reactor-4 along with a 15.5 M feed of NaOH, producing neodymium hydroxide. The reactor was set to operate at 100 °C and 10 atm. Similarly to the reaction taken place in reactor-2, sodium sulfate was also produced as a byproduct of the reaction and had to be hydrolyzed by a water feed in mixer 2 (Mix-2). Once the sodium sulfate was hydrolyzed out, the stream (S-30) was fed into filter-5 where Nd(OH)₃ was separated from the aqueous waste resulting in a pure Nd(OH)₃ stream (S-32). Finally, the isolated hydroxide would be fed into a calciner converting the hydroxide into the target product, neodymium oxide. OLI does not simulate calciners so calculations were made by hand to estimate cost for a calciner, the calculations can be found in appendix C.6.

4.2.7 Water Recycle Stream 2

The aqueous stream leaving filter-5 (S-31) contains no products to be isolated and is to be treated as waste and sent to a waste neutralizer. Before this, the stream is sent to a separator (Sep-2) to recover the water left in the stream. The stream is conditioned by a pump (Pump-2) and heat exchanger (heat exch-4) to raise the temperature and pressure of the stream to 220 °C and 15 atm. At these conditions, 20,720 mol/hr of water is recovered (S-33) that can then be sent through the system to be utilized. The aqueous stream (S-34) is then treated as a waste stream and sent to be neutralized.

4.2.8 Waste Neutralization

There are four streams in the system that are treated as waste streams: S-9, S-17, S-25 and S-34. The components of which comprise mainly of water, leftover reactants and trace amounts of unrecovered rare earth elements, with the exception of unwanted cerium and lanthanum sulfates from S-17. These streams are all combined into S-37 with a pH of 0.364, to be properly disposed and/or sent for treatment, the pH of the stream must be brought to more neutral conditions. S-37 is fed into a neutralizer (Neutrl-1) where a 20.6 M solution of NaOH is used to bring the pH of the final combined waste stream to neutral conditions.

4.3 Safety, Health, and Environmental Analysis

The environmental health, and safety effects of the chemical process are into account when designing the extraction process. The things that are considered are stream hazards, environmental pollution, and finally health and safety of the workers. In consideration for the stream hazards a stream hazard chart was drawn up reference Table III. In order to mitigate some of these hazards we look to equipment design. First, in order to handle some of the corrosive materials we must design the equipment with materials that can handle such compounds. Pressure and temperature should be monitored in order to maintain safe conditions for the compounds. Finally, routine maintenance should be conducted to ensure that hazardous compounds are not leaking due to equipment failure. The risk of these hazards to the safety and health of the community and environment should be minimized through compliance with the federal regulation. In order to reduce pollution several risks must be considered; these risks are wastewater streams and radon gas emission. Wastewater streams are recycled as well neutralized within our process; we work to reduce some of the pollution; however, further consideration should be taken for the waste stream to be fully safe to release. Radon gas is a known carcinogen that results from the process of thorium decay. In order to reduce this risk radon detectors should be set up and proper ventilation should be employed. In terms of the necessary equipment for proper ventilation,

radon capture systems have been incorporated to absorb the radon from the areas where thorium decay may occur. For worker safety, the main concerns are due to the hazardous nature of the stream materials. First, in order to reduce the risks of the stream hazards to employees is to ensure that all employees are informed of the properties of the process chemicals. This should take place in the form of a required chemical safety training provided to process employees. Second, process employees are to be provided with the appropriate personal protective equipment. All process employees should wear closed-toe shoes, long sleeves shirts, eye protection, and gloves at all times when working near the process equipment. Finally, to protect process employees the thorium-recovery process plant should be equipped with an appropriate amount of ventilation, eye wash stations, chemical showers, and first-aid kits to be used in the case of an emergency.

Table III. Safety hazards chart.

Materials	MW	Melting Point C	Flash Point C	Boiling Point C	Liquid Density Kg/m ³	Flammability	Deadly Posion	Toxin	Carcinogenic	Mutagenic	Irratating	Corrosive
ThO ₂	264.04	3390	-	4400	10	non	no	yes	presumed	yes	yes	no
H ₂ SO ₄	98.08	10	-	290	1.84	non	no	yes	no	no	yes	yes
Th(SO ₄) ₂	424.16	200	-	-	2.8	non	no	yes	-	-	yes	yes
NH ₄ OH	35.04	-69	-	27	0.91	non	no	yes	no	yes	yes	yes
NH ₃	17.03	-72	-	36	0.9	non	no	yes	-	-	yes	yes
SO ₃	80.07	16.8	-	44.8	1.92	non	presumed	yes	yes	-	yes	yes
CePO ₄	235.09	-	-	-	5.22	non	no	yes	-	-	yes	no
Ce ₂ (SO ₄) ₃	568.42	-	-	-	-	-	-	-	-	-	yes	yes
LaPO ₄	236.89	-	-	-	-	non	no	yes	-	-	yes	no
La ₂ (SO ₄) ₃	565.99	1150	-	-	2.8	non	no	yes	-	-	yes	yes
Nd ₂ (SO ₄) ₃	576.7	1176	-	-	2.85	non	no	yes	-	-	yes	yes
NdPO ₄	239.21	-	-	-	-	non	no	yes	-	-	yes	no
NaOH	40	318	-	1390	-	non	-	-	-	-	yes	yes
La(OH) ₃	189.9	~2000	-	~4000	4.28	non	no	yes	-	-	yes	yes
Ce(OH) ₃	191.14	~2001	-	~4001	6.77	non	no	yes	-	-	yes	yes
(P ₂ O ₅) ₂	141.94	340	-	360	2.39	non	no	yes	-	-	yes	yes
Na ₂ SO ₄	142	880	-	1700	2.68	non	no	yes	yes	yes	yes	no
(NH ₄) ₂ SO ₄	132.1	280	-	-	-	non	no	-	-	-	yes	-
Ce ₂ O ₃	328	3730	-	-	6.2	non	no	yes	-	-	yes	no
H ₂ O	18.1	0	-	100	1	non	no	no	no	no	no	no
Na ₄ P ₂ O ₇	265.9	80	-	93.8	-	Yes	no	-	yes	-	yes	-
La ₂ O ₃	325.81	2315	-	4200	6.51	non	no	yes	-	-	yes	no
Nd(OH) ₃	163.2652	~2000	-	~4000	-	non	no	yes	-	-	yes	yes
Nd ₂ O ₃	336.48	2270	-	-	7.24	non	no	yes	-	-	yes	no

4.3.1 Water recycle

In order to reduce the cost of the process as well as to be environmentally responsible, multiple water recycle streams were implemented in the largest waste streams of the process. Separator 1 was implemented as a way to recover water and sulfuric acid from the reactor that processes neodymium. Recovering water and sulfuric acid both reduces the amount spent on materials and reduces the amount of energy to operate a heat exchanger to prepare the stream for separation. The separator was able to remove 17.028 kmol/hr of utilizable water vapor, as well as a stream consisting of 8.970 kmol of sulfuric acid and 4.229 kmol/hr of water which can be recycled into stream S-15. Another water recovery system was implemented after the neodymium recovery process. This separator recovered 20.720 kmol/hr of water. Due to the limitations in OLI, neutralizers need a significant amount of water in order to converge. This requirement limits the amount of water that can be recovered in simulations in OLI. Simulating the process in other softwares could provide a better understanding of the amount of water that can be removed from the process safely.

4.4 Capital Cost Estimates

Volumetric flow rates provided by the OLI software were used to size the equipment. Molar flow of each species and mass flow of each stream can be found in Appendix A. Temperature, pressure, and fluid properties such as corrosivity were considered in material selection for each piece of equipment. Because of the high corrosivity of the acidic solutions used, stainless steel was selected for all equipment. The equipment needed for this process includes: four heat exchangers, four reactors, one neutralizer, three mixers, five filters, two separators, one calciner, one rotary kiln, one component splitter, and two pumps. The most recent CEE Index value for 2021 of 595.9 is used in equipment costing. Using the EconExpert program developed by P.T. Vasudevan and T. Ulrich and reference values from 2004 (CEE index value of 400), the cost of each piece of equipment is determined. A table of equipment for this process is shown below in Table IV.

Table IV. Equipment list.

EQUIPMENT LIST	
Equipment Type	Quantity
Heat Exchanger	4
Reactors	4
Neutralizer	1
Mixer	3
Separators/Filters	6
Calciner	1
Splitter	1
Pumps	2
Rotary Kiln	1
Carbon Adsorber	1

A detailed breakdown of the equipment list can be found in Appendix B. For the heat exchangers, the heat duty and log mean temperature difference provided by OLI along with an overall heat transfer coefficient found in the literature are needed to calculate the area. This area is the important parameter for overall heat exchanger price. For the reactors, the heat duty and an assumed residence time are required to determine the minimum volume of the reactor. A safety factor of three is included to ensure the reactors can handle any additional volume. The required volume is then used to price the reactors. Filters and mixers use the heat duty provided by OLI and an assumed residence time and height to determine the filter diameter and the diameter of the mixer. The diameter of the filter is used to determine the filter area in order to price the equipment. The diameter of the mixer is used to determine its price. Both the filter and mixer sizes also include a safety factor of three. To size the neutralizers, the heat duty and an assumed residence time are required to determine the minimum volume. Again, a safety factor of three is included to determine the required volume. This volume is used to price the neutralizers. To size the calciner, the heat duty and residence time are needed to determine the volume. A safety factor of three is also implemented for the calciner. The rotary kiln was priced in the same manner as the calciner. The component splitter was priced as a vertical-oriented process vessel. The height, diameter, residence time, and volumetric flow rate were used to price this piece of equipment. The carbon

adsorber was also priced as a vertically-oriented process vessel. This also included activated carbon as the packing material. A vessel and packed height and residence time are used to determine the diameter which is important in pricing the equipment. For the pumps, power usage was provided by OLI. This value and the pressure were needed to cost the pumps. All equipment except for the carbon adsorber was designed using stainless steel as this was the proper material for the corrosivity of the process. The carbon adsorber was designed using carbon steel. Detailed example calculations for equipment sizing and costing can be found in Appendix C. The total bare module cost of equipment for this process was determined to be \$6.8 million. Including contingency, fees, and auxiliary facilities, the grass roots capital sums to \$10.5 million. The capital cost summary table is shown below in Table V.

Table V. Capital cost summary.

Job title: Thorium Dioxide Extraction		Cost Index Type <u>AICHE Index</u>		Cost Index Value <u>595.9</u>			
Equipment Identification	Number	Capacity or Size Specifications	Total Purchased Cost, C _{BM}	Bare Module Factor OR Material Factor	Pressure, F _p	Actual Bare Module Cost, C _{BM}	Total
Heat Exchangers							
Heat Exchanger 1	HX-1	2.03 m ² , stainless steel, U-tube, 10 barg	\$ 3,905.0	3.0	1.0	\$ 22,579.00	
Heat Exchanger 2	HX-2	0.1 m ² , stainless steel, U-tube, 10 barg	\$ 3,905.0	3.0	1.00	\$ 22,579.00	
Heat Exchanger 3	HX-3	0.25 m ² , stainless steel, U-tube, 10 barg	\$ 3,905.0	3.0	1.00	\$ 22,579.00	
Heat Exchanger 4	HX-4	30.6 m ² , stainless steel, U-tube, 15 barg	\$ 9,279.0	3.0	1.03	\$ 54,824.00	
Total Heat Exchangers	4.000		\$ 20,994.0				\$122,561
Reactors							
Reactor 1	R-1	3.2 m ³ , stainless steel, 15 barg	\$ 12,071.0	7.5	1.64	\$ 148,453.00	
Reactor 2	R-2	455.8 m ³ , stainless steel, 15 barg	\$ 234,194.0	7.5	1.64	\$ 2,880,175.00	
Reactor 3	R-3	9.8 m ³ , stainless steel, 15 barg	\$ 19,246.0	7.5	1.64	\$ 236,693.00	
Reactor 4	R-4	2.3 m ³ , stainless steel, 10 barg	\$ 10,900.0	7.5	1.38	\$ 113,061.00	
Reactor Total	4.000		\$ 276,411.0				\$3,378,382
Seperators and Filters							
Filter 1	F-1	1.59 m ³ , stainless steel	\$ 11,291.0	3.6	-	\$ 40,648.00	
Filter 2	F-2	0.64 m ³ , stainless steel	\$ 7,876.0	3.6	-	\$ 28,354.00	
Filter 3	F-3	3.78 m ³ , stainless steel	\$ 18,892.0	3.6	-	\$ 68,012.00	
Filter 4	F-4	0.13 m ³ , stainless steel	\$ 7,876.0	3.6	-	\$ 28,354.00	
Filter 5	F-5	1.68 m ³ , stainless steel	\$ 11,645.0	3.6	-	\$ 41,920.00	
Separator 1	S-1	211.49 m ³ , stainless steel	\$ 46,128.0	3.6	-	\$ 166,061.00	
Separator 2	S-2	158.48 m ³ , stainless steel	\$ 37,543.0	3.6	-	\$ 135,154.00	
Total Filters and Separators	7.000		\$ 141,251.0				\$508,503
Mixers							
Mixer 1	M-1	0.4 m diameter, stainless steel	\$ 16,648.0	2.9	-	\$ 48,279.00	
Mixer 2	M-2	0.64 m diameter, stainless steel	\$ 23,359.0	2.9	-	\$ 67,741.00	
Mixer 3	M-3	0.64 m diameter, stainless steel	\$ 23,359.0	2.9	-	\$ 67,741.00	
Total Mixers	3.000		\$63,366				\$183,761
Neutralizers							
Neutralizer 1	N-1	1.32 m ³ , stainless steel, horizontal bullet tank, 10 barg	\$ 5,638.0	3.8	-	\$ 21,425.00	
Total Neutralizers	1.000		\$5,638				\$21,425
Calciners							
Cacliner 1	C-1	0.10 m ³ , rotary kiln, stainless steel	\$ 142,458.0	4.5	-	\$ 641,063.00	
Total Calciners	1.000		\$142,458				\$641,063
Rotary Kiln							
Rotary Kiln 1	RK-1	5.72 m ³ , rotary kiln, stainless steel	\$ 140,102.0	6.0	-	\$ 840,609.00	
Total Rotary Kiln	1.000		\$140,102				\$840,609
Component Splitter							
Component Splitter 1	CS-1	0.62 m diameter, 10 m height, 15 barg, stainless steel	\$ 29,616.0	4.0	1.9	\$ 456,611.00	
Total Component Splitter	1.000		\$29,616				\$456,611
Carbon Adsorber							
Carbon Adsorber 1	CA-1	2.76 m diameter, 15 m height, carbon steel, activated carbon packing	\$ 214,390.0	1.0	1.0	\$ 563,027.00	
Total Carbon Adsorber	1.000		\$214,390				\$563,027
Pumps							
Pump 1	P-1	2 kW, stainless steel, rotary positive displacement	\$ 10,448.0	2.0	1.0	\$ 52,004.00	
Pump 2	P-2	0.29 kW, stainless steel, rotary positive displacement	\$ 5,238.0	2.0	1.2	\$ 29,419.00	
Total Pumps	2.000		\$15,686				\$81,423
Total bare module cost			Base materials, C _{TBM} = $\sum C_{BM}$ =		Actual materials, C _{TBM} = $\sum C_{BM}$ =		\$6,797,365
Contingency and fee					C _C + C _F = C _{TBM} × 0.18 =		\$1,223,526
Total module cost					C _{TM} =		\$8,020,891
Auxiliary (offsite) Facilities					C _{TBM} × 0.30 =		\$2,406,267
Grass Roots capital					C _{GR} =		\$10,427,158

*2004 cost x (Target Year Cost Index/2004 Cost Index)

Figure 4 below shows the distribution of equipment costs for the entire process. As shown, the reactors encompass half of the equipment cost. The rotary kiln, calciner, carbon adsorber, and component splitter are also costly pieces of equipment. The mixers, neutralizer, pumps, and separators and filters are minimal costs in comparison.

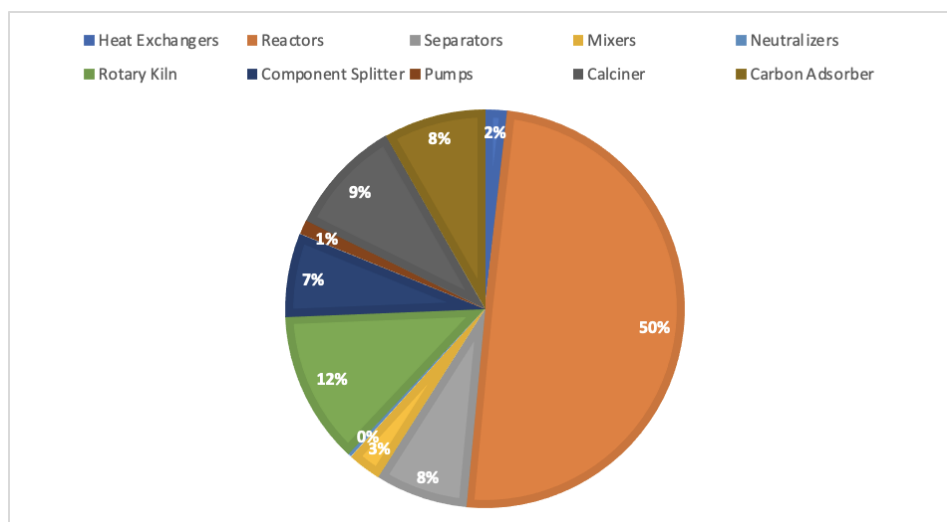


Figure 4. Capital cost distribution.

4.5 Manufacturing Cost Estimates

Manufacturing costs are determined based on the fixed capital cost. The total capital investment is the fixed capital cost combined with the working cost, which is around 15% of the fixed capital cost. Manufacturing expenses include raw materials, solvents, operating labor, clerical labor, utilities, maintenance and repairs (~6% of fixed capital), operating supplies (~15% of maintenance and repairs), laboratory charges (~15% of operating labor), and patents and royalties (~3% of total expense). Utility usage is determined from values provided by OLI software. Utilities needed for this process include electricity, cooling water, and steam. Realistically, natural gas will likely also be utilized; however, this is not accounted for in this economic analysis. Indirect manufacturing expenses include overhead, packaging, and storage, local taxes, and insurance. Indirect expenses account for the smallest percentage of manufacturing costs. In addition to

manufacturing expenses and indirect expenses, there are general expenses constituting administrative costs (~25% of overhead), distribution and selling (~10% of total expense), and research and development (~5% of total expense). Depreciation is anticipated to be approximately 10% of the fixed capital. Including all of these expenses, the total manufacturing expenses equate to \$15.2 million. However, when byproducts are included, the manufacturing expenses end up negative. This is because the value of the byproducts outweigh the price of the manufacturing expenses. Therefore, a net of almost \$3.8 million are saved in manufacturing expenses. The price of thorium dioxide was determined to be \$776,000 per kg, resulting in a revenue from sales of \$37.7 million. This results in a net annual profit after taxes of \$26.2 million. A detailed manufacturing cost summary can be seen below in Table VI.

Table VI. Manufacturing cost summary.

MANUFACTURING COST SUMMARY									
Job Title: Thorium Dioxide Extraction									
Cost Index Type: AICHE Index Cost Index Value: 595.9									
Capital									
Fixed capital, C_{FC}	\$	8,020,890.70							
Working capital (10-20% of fixed capital), C_{WC}	\$	1,203,133.61							
Total capital investment, C_{TC}	\$	9,224,024.31							
Manufacturing Expenses									
Direct									
Raw materials						\$/yr		Unit Price \$/m ³	
By-product credits						\$			
Catalysts and solvents						\$			
Operating labor						\$			
Supervisory and clerical labor (10-20% of operating labor)						\$			
Utilities									
Steam	148219200.00	kg/y		33	barg @	\$	0.02	\$/kg	
Electricity	18,777.92	kWh @	\$	0.12	\$/kWh	\$			
Process water	6,930.48	m ³ @	\$	0.89	\$/m ³	\$			
Demin water		m ³ @			\$/m ³				
Cooling water	148,219.20	m ³ @	\$	0.07	\$/m ³	\$			
Waste disposal		kg @			\$/kg				
Maintenance and repairs (2-10% of fixed capital)						\$			
Operating supplies (10-20% of maint & repairs)						\$			
Laboratory charges (10-20% of operating labor)						\$			
Patents and royalties (0-6% of total expense)						\$			
Total, A_{DME}						\$	(3,806,242.15)	\$	(78,320.80)
Indirect									
Overhead (payroll and plant), packaging, storage (50-70% of op. Labor+supervision+ maint.)						\$			
Local taxes (1-3% of fixed capital)						\$			
Insurance (1-2% of fixed capital)						\$			
Total, A_{ME}						\$	650,927.64	\$	13,394.10
Total manufacturing expense, $A_{ME} = A_{DME} + A_{ME}$									
General Expenses									
Administrative costs (25% of overhead)						\$			
Distribution and selling (10% of total expense)						\$			
Research and development (5% of total expense)						\$			
Total general expense, A_{GE}						\$	(306,393.77)	\$	(6,304.65)
Depreciation (approximately 10% of fixed capital), A_{BD}									
Total Expenses, A_{TE}						\$	(2,659,619.21)	\$	(54,726.82)
Revenue from Sales	48.59809822	m ³ /yr @	\$	776,000.00	\$/m ³ , A_s	\$	37,712,124.22	\$	776,000.00
Net annual profit, A_{NP}						\$	40,371,743.43	\$	830,726.82
Income taxes (net annual profit times the tax rate), A_{IT}						\$	14,130,110.20	\$	290,754.39
Net annual profit after taxes ($A_{NP} - A_{IT}$), A_{NNP}						\$	26,241,633.23	\$	539,972.43
Aftertax rate of return, $i = (1.5 A_{NNP}/C_{TC}) \times 100 =$									
426.74 %									

A distribution of manufacturing costs can be seen below in Figure 5. As shown, the bulk of the manufacturing costs stem from the purchasing of raw materials and reactants such as monazite, NaOH, H₂SO₄, H₃PO₄, and water. The utility usage also accounts for a large portion of the manufacturing costs. The utility usage for this process is based on the heat duties of each piece of equipment as provided by OLI. Likely some of this equipment would be powered by natural gas, increasing the cost of natural gas usage and thus utility price. The price of raw materials is expected to remain a large portion of the manufacturing costs. The selling of byproducts such as neodymium oxide and phosphorus pentoxide greatly decreases the direct manufacturing expenses, making this process highly profitable.

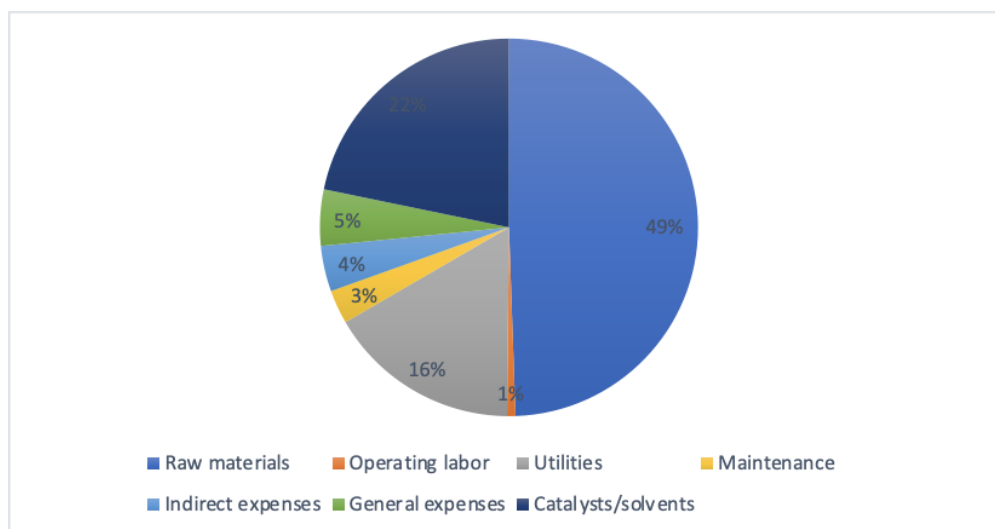


Figure 5. Distribution of manufacturing costs.

5.0 Discussion of Results

The separation process of thorium from monazite ore was successfully simulated in OLI software. Through the use of a rotary kiln to convert the rare earth phosphates in monazite into rare earth sulfate forms, a separator to separate the thorium sulfate, a reactor to convert the thorium sulfate into thorium dioxide and a separator to retrieve the thorium dioxide, thorium was recovered with a recovery rate of 99.8%. The stream of other rare earth elements was processed to separate phosphorus pentoxide, cerium, lanthanum, and

neodymium. Phosphorus pentoxide was also recovered at a rate of 3.53 kmol/hr. In OLI extractors are difficult to simulate, therefore an idealized version of the separation was used by adding a component splitter. This component splitter would be replaced by an extractor and the manufacturing cost has been adjusted accordingly. Cerium and lanthanum were attempted to be recovered in OLI, but the cost to recover was higher than the profits of selling the metals, therefore they were discarded in a waste stream. Neodymium was recovered in a similar manner to thorium, but OLI is not able to simulate the last step in the recovery of neodymium. A calciner is needed to convert the neodymium hydroxide into neodymium oxide. The percent recovery of neodymium from the separation was 95.7% which should not change after being processed by a calciner. A calciner has been priced for the process, however a simulation has not been conducted to predict the resulting product composition. The process does use a significant amount of water and produces a significant amount of waste. An effort was made to reduce the amount of waste early on, but there is room for improvement.

The capital costs from this process primarily are greatly increased in this process due to the need for stainless steel equipment. The manufacturing expenses are dominated by utility and raw material expenses. Incorporated all capital and manufacturing costs, the net annual profit after taxes expected for this process is over \$26.2 million. This results in an after-tax rate of return of 427%.

6.0 Conclusions

A process design of thorium dioxide extraction from monazite ore with profitable byproducts was successfully produced using the OLI software. The economic analysis shows that this process can be highly profitable by the selling of byproducts including neodymium oxide and phosphorus pentoxide. Based on the economic analysis, the net annual profit after taxes is over \$26.2 million with an after-tax rate of return of 427%. This is likely not realistic as many assumptions were made in this design. Even though our estimates

were conservative, the realistic capital and manufacturing costs of this facility would almost certainly be higher. While an effort was made to optimize the reagents used, further optimization could be done to reduce costs as well as reduce waste. The reactants such as H_2SO_4 are corrosive and would greatly increase the maintenance costs that we determined. Moreover, only equipment prices and utilities were accounted for in the economic design; production of the physical facility itself was not included. In addition, the byproducts were priced based on their pure forms; however the phosphorus pentoxide is in a mixed stream. By including all of these unaccounted for costs, the process would produce a much more reasonable profit and rate of return.

7.0 Recommendations

While the proposed process for refining thorium is feasible, there are a number of factors that should be considered before implementation. OLI has been an invaluable resource in process drafting, but there are a few areas where it falls short. There is no easy way to automatically optimize a feed stream for a reaction. Another problem is that OLI requires a significant amount of water for reactors to converge. Lastly reactions will sometimes be simulated in process blocks that might not realistically support a reaction. The utilization of a different software, along with smaller scale experiments may be needed to fully optimize the process.

One recommendation regarding design is in reactors 2 and 4, using ammonium hydroxide in place of sodium hydroxide would avoid the byproduct precipitation of sodium sulfate and result in less water needed when isolating ThO_2 and $\text{Nd}(\text{OH})_3$.

The recommendations laid out within the safety, health, and environmental analysis are crucial to the safety of the workers, community, and environment. Thus, these recommendations should be considered in the construction of any monazite processing facility

In order to reduce cost as well as reduce waste the amount of sodium hydroxide, water, and sulfuric acid should be reduced when possible. Reducing the amount of material will reduce material costs, as well as reduce the amount of energy required for temperature and pressure changes throughout the process. Optimizing the water recovery step will also help to reduce costs as well as reduce the environmental impact of the process.

8.0 References

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9.0 Appendices

Appendix A: Mass and Molar Flow Rates by Stream

The flow rates provided by OLI in kmol/hr for each species are specified. The total mass flow rates in kg/hr and total volumetric flow rates in m³/kg for each stream are also specified in the following tables.

Table A.I. Flow rates for stream 0a through 15.

Compound	MW (kg/kmol)	Stream (kmol/hr)														
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
ThO ₂	264.04			0.0005789		0.00057893		0.216815	0.216815	1.04E-14	0.216815		1.47E-09		0.216815	
H ₂ SO ₄	98.08							3.58E-36								9.50E+00
Th(SO ₄) ₂	424.16	0.217394		0.216815	216.815								0.000578929			
NH ₄ OH	35.04															
NH ₃	17.03															
SO ₃	80.07			4.13416		4.13416		0.0540016		0.43363	0.117795		0.0086865		0.43363	
CePO ₄	235.09															
Ce ₂ (SO ₄) ₃	568.42	0.720145											0.719388			
LaPO ₄	236.89			0.726023		0.726023										
La(SO ₄) ₃	565.99												0.363012			
Nd ₂ (SO ₄) ₃	576.7	0.29451											0.292371			
NdPO ₄	239.21			0.589019		0.589019										
NaOH	40						0.9	0.140743		0.9	0.268331				0.9	
La(OH) ₃	189.9															
Ce(OH) ₃	191.14															
(P ₂ O ₅) ₂	283.88											1.50094				
P ₂ O ₅	141.945			2.87563		2.87563						0.531263				
Na ₂ SO ₄	142							0.379629			0.315835					
(NH ₄) ₂ SO ₄	132.1															
Ce ₂ O ₃	328			0.720145		0.720145							0.000756714			
H ₂ O	18.1	4.6		18.4666		18.4666	2	2.37963		8	2.31583	1.87391	16.5862	6	8	7
CePO ₄ ·2H ₂ O	271.12															
LaPO ₄ ·2H ₂ O	269.91															
NdPO ₄ ·2H ₂ O	275.24															
Na ₄ P ₂ O ₇	265.9															
La ₂ O ₃	325.81															
Nd(OH) ₃	163.2652												0.00427757			
Na ₃ PO ₄ ·1H ₂ O	181.96															
Nd ₂ (SO ₄) ₃ ·8H ₂ O	720.78															
La ₂ (SO ₄) ₃ ·9H ₂ O	728.1363	0.363012														
H ₃ PO ₄	97.994	2.0663		5												
Nd ₂ O ₃	336.48															
Total Flow Rate (kg/hr)		1.22E+03	4.90E+02	1.71E+03	9.20E+04	1.62E+03	7.22E+01	1.64E+02	5.72E+01	2.16E+02	1.64E+02	5.35E+02	1.71E+03	1.09E+02	2.73E+02	1.06E+03
Total Volumetric Flow Rate (m³/hr)		2.61E-01	0.521044	0.0217661	0.499278	3.39E-02	32.6106	0.0058061	0.167678	0.0711977	0.246766	0.521044	1.09E-01	0.173484		

Table B.II. Equipment list with sizing and utility needs for neutralizers, splitter, calciner, rotary kiln, carbon adsorber, and pumps.

Job title: Thorium Dioxide							
Equipment Type							
EQUIPMENT LIST-- Thorium Dioxide	Neutralizer	Splitter	Calciner	Rotary Kiln	Pumps		Carbon Adsorber
Number	N-1	CS-1	C-1	RK-1	P-1	P-2	CA-1
Stream Number	37	5	32	1	18	31	All thorium streams
Temperature (°C)	In	107.509	200				
	Out	107.509	200				
Pressure (barg)	In	0.0	14.1855		4.053	0.0	
	Out	0.0	14.1855		9.11925	14.1855	
Flow rate: Mass (kg/s)	0.30	0.45	0.03	0.34	0.43	0.16	
Volumetric (m ³ /s)	4.56E-02	1.39E-04	4.22E-06	2.65E-04	2.55E-03	1.30E-04	5.00E-02
Ave. Density (kg/m ³)	1240.98	3242.87	7.24E+03	1281.26	1.67E+02	1.23E+03	
Stream Number							
Name							
Process Orientation							
Phase							
Temperature (°C)	In						
	Out						
Pressure (barg)	In						
	Out						
Flow rate: Mass (kg/s)							
Volumetric (m ³ /s)							
Ave. Density (kg/m ³)							
Ave. Heat Capacity (kJ/kg°C)							
Heat-Transfer Coefficient (J/m ² s°C)							
Efficiency (%)							
Heating duty (kJ/s)							
LMTD (°C)							
F _r							
ΔT _m = MTD x F _r (°C)							
Utilities							
Electricity (kW)					1.99475	0.285674	
Cooling water (m ³ /s)							
Fuel							
Steam (kg/s)							
(Pressure (bara))							
Equipment Size							
Length or height, L (m)							
Width or diameter, D (m)		0.62					
Surface area, A (m ²)							
Volume, V (m ³)	1.32	3.00	0.09	5.72			2.76
Design Pressure (barg)		15			10	15	90.00
Shaft power, w _s (kW)					1.99475	0.285674	1
Physical orientation							Vertical
Material of construction	stainless steel	stainless steel	stainless steel	stainless steel	stainless steel		carbon steel
Other specifications							activated carbon packing

Appendix C: Equipment Sizing and Costing Example Calculations

The Ulrich method was used to price and size each equipment. The EconExpert software developed by P.T. Vasudevan and T. Ulrich and reference values were used to price equipment as well. Reference values are from 2004 (CEE index value of 400). The CEE Index value of 595.9 for 2021 was used to price the equipment. Values provided by the OLI software were also used for sizing the equipment. Some additional values were gathered from the literature or based on assumptions supported by literature. All equipment was priced based on stainless steel as the material.

1. Heat Exchanger-1

The heat exchangers were all determined to be shell and tube heat exchangers made from stainless steel. OLI provided mass flow rates and temperatures of the incoming and outgoing streams. An overall heat transfer coefficient was determined from other sources. Combining all of the parameters in the calculations below, a heat exchanger area can be determined which is necessary in pricing the equipment.

Parameters: $U = 1000 \text{ (J/m}^2\text{s}^*\text{C)}$; $T_{Hi} = 57 \text{ C}$; $T_{Ho} = 40 \text{ C}$; $T_{Ci} = 0 \text{ C}$; $T_{Co} = 50 \text{ C}$

$$\Delta T_{LM} = \frac{(T_{Hi} - T_{Co}) - (T_{Ho} - T_{Ci})}{\ln\left(\frac{T_{Hi} - T_{Co}}{T_{Ho} - T_{Ci}}\right)} = \frac{(57-50) - (40-0)}{\ln\left(\frac{57-50}{40-0}\right)} = 23.8 \text{ C}$$

$$A = - \frac{Q}{\Delta T_{LM} * U} = - \frac{\frac{Q}{3600}}{23.8 * 1000} = 2.03 \text{ m}^2$$

Using EconExpert, total purchased cost = \$3,905.

$F_m(\text{carbon steel}) = 3.0$; $F_p(P = 10 \text{ barg}) = 1.0$

$$C_{BM,HE1} = F_{BM} * \$3,905 * \left(\frac{595.9}{400}\right) = \$22,579$$

2. Reactor-1

A typical residence time of 2 hours (7200 seconds) was selected for the reactors. Upon a more detailed design, this may change and affect the price of the reactors. However, to account for this, a factor of 3 was used to increase the volume so that the reactors should be able to handle up to three times the expected volume. The OLI software provided the volumetric flow rate. The volume can then be calculated and used to price the carbon steel reactors.

Parameters: $Q = 0.000147 \text{ m}^3/\text{s}$; residence time = 2 hrs = 7200 seconds

$$\text{Volume} = \text{residence time} * Q * \text{factor of 3} = 7200 \text{ s} * 0.000147 \frac{\text{m}^3}{\text{s}} * 3 = 3.2 \text{ m}^3$$

Using EconExpert, total purchased cost = \$12,071.

$F_{bm}(\text{stainless steel}) = 7.5$; $F_p(P = 15 \text{ barg}) = 1.64$

$$C_{BM,R1} = F_{BM} * \$12,071 * \left(\frac{595.9}{400}\right) = \$148,453$$

3. Filter-1

A typical residence time of one hour (3600 seconds) was selected for the filters. This was used along with the volumetric flow rate provided by OLI to calculate the minimum volume. Again, a factor of 3 was used to size up the filters so that any necessary volume could be contained. Assuming a cylindrical shape and setting the height equal to 1 meter, diameters were then calculated for the filters. The height assumed for the separators was 15 meters. These diameters were used to price the stainless steel filters/separators.

Parameters: $Q = 0.000145 \text{ m}^3/\text{s}$; residence time = 1 hr = 3600 seconds; $H = 1 \text{ m}$

$$Volume = 3600 \text{ s} * 0.000145 \frac{\text{m}^3}{\text{s}} * 3 = 1.59 \text{ m}^3$$

$$D = \sqrt{\frac{4*V}{\pi*H}} = \sqrt{\frac{4*1.59}{\pi*1}} = 1.42 \text{ m}$$

Using EconExpert, total purchased cost = \$11,291.

$$F_{bm}(\text{stainless steel}) = 3.6$$

$$C_{BM,F1} = F_{BM} * \$11,291 * \left(\frac{595.9}{400}\right) = \$40,648$$

4. Mixer-1

The volumetric flow rate provided by OLI and a typical residence time of 30 minutes (1800 seconds) was used to calculate the mixer volume. Assuming a cylindrical shape and a height of 10 meter, the minimum mixer diameter was calculated. Again, a factor of 3 was used as a safety precaution. The diameter was used to price the mixers.

Parameters: $Q = 0.0000591 \text{ m}^3/\text{s}$; residence time = 2 hours = 7200 seconds; $H = 10 \text{ m}$

$$Volume = 7200 \text{ s} * 0.0000591 \frac{\text{m}^3}{\text{s}} * 3 = 1.28 \text{ m}^3$$

$$D = \sqrt{\frac{4*V}{\pi*H}} = \sqrt{\frac{4*1.28}{\pi*10}} = 0.40 \text{ m}$$

Using EconExpert, total purchased cost = \$16,648.

$$F_{bm}(\text{stainless steel}) = 2.9$$

$$C_{BM} = F_{BM} * \$16,648 * \left(\frac{595.9}{400}\right) = \$48,279$$

5. Neutralizer-1

The neutralizers were sized as bullet vessels as they essentially are a vessel where two streams enter and neutralize each other until they can be safely disposed of. A residence time of 30 minutes (1800 seconds) is assumed. Again, a factor of three is used to ensure the neutralizer can contain any extra volume. This volume is then used to price the equipment.

Parameters: $Q = 0.0465 \text{ m}^3/\text{s}$; residence time = 30 minutes = 1800 seconds

$$Volume = residence\ time * Q * factor\ of\ 3 = 1800\ s * 0.0465 \frac{\text{m}^3}{\text{s}} * 3 = 1.32 \text{ m}^3$$

Using EconExpert, total purchased cost = \$5,638.

$$F_{bm}(stainless\ steel) = 3.8$$

$$C_{BM} = F_{BM} * \$5,638 * \left(\frac{595.9}{400}\right) = \$21,425$$

6. Calciner-1

Using the volumetric flow rates provided by OLI and an assumed residence time of two hours (7200 seconds), a volume can be calculated. A factor of three is used to ensure the calciner can handle any additional volume safely.

Parameters: $Q = 0.00000422 \text{ m}^3/\text{s}$; residence time = 2 hours = 7200 seconds

$$Volume = residence\ time * Q * factor\ of\ 3 = 7200\ s * 0.00000422 \frac{\text{m}^3}{\text{s}} * 3 = 0.10 \text{ m}^3$$

Using EconExpert, total purchased cost = \$142,458.

$$F_{Bm}(stainless\ steel) = 4.5$$

$$C_{BM} = F_{BM} * \$142,458 * \left(\frac{595.9}{400}\right) = \$641,063$$

7. Rotary Kiln-1

Using the volumetric flow rates provided by OLI and an assumed residence time of two hours (7200 seconds), a volume can be calculated. A factor of three is used to ensure the rotary kiln can handle any additional volume safely.

Parameters: $Q = 0.000265 \text{ m}^3/\text{s}$; residence time = 2 hours = 7200 seconds

$$\text{Volume} = \text{residence time} * Q * \text{factor of 3} = 7200 \text{ s} * 0.000265 \frac{\text{m}^3}{\text{s}} * 3 = 5.72 \text{ m}^3$$

Using EconExpert, total purchased cost = \$140,102.

$$F_{Bm}(\text{stainless steel}) = 6.0$$

$$C_{BM} = F_{BM} * \$142,458 * \left(\frac{595.9}{400}\right) = \$840,609$$

8. Pump-1

The pumps were priced as positive displacement rotary pumps. Power usage and pressure were provided by the OLI software. These values were used to calculate the total price of each pump.

Parameters: $Q = 0.00255 \text{ m}^3/\text{s}$; power = 1994.75 J/s = 2.0 kW; $p = 10 \text{ barg}$

Using EconExpert, total purchased cost = \$10,448.

$$F_{Bm}(\text{stainless steel}) = 2.0; F_p(10 \text{ barg}) = 1.0$$

$$C_{BM} = F_{BM} * \$10,448 * \left(\frac{595.9}{400}\right) = \$52,004$$

9. Component Splitter-1

The component splitter was priced as a vertically-oriented process vessel with no packing or trays. A residence time of 2 hours was assumed in order to calculate the volume required. This volume is multiplied by a factor of 3 to ensure safety. A diameter can then be calculated using a height of 10 meters. This diameter and height are used to calculate the equipment cost.

Parameters: $Q = 0.000139 \text{ m}^3/\text{s}$; residence time = 2 hours = 7200 seconds; $H = 10 \text{ m}$

$$\text{Volume} = 7200 \text{ s} * 0.000139 \frac{\text{m}^3}{\text{s}} * 3 = 3.00 \text{ m}^3$$

$$D = \sqrt{\frac{4*V}{\pi*H}} = \sqrt{\frac{4*3}{\pi*10}} = 0.62 \text{ m}$$

Using EconExpert, total purchased cost = \$29,616.

$$F_{bm}(\text{stainless steel}) = 4.0; F_p = 1.87$$

$$C_{BM} = F_{BM} * \$29,616 * \left(\frac{595.9}{400}\right) = \$456,611$$

10. Carbon Adsorber-1

The carbon adsorber for radon mitigation was priced as a vertically-oriented process vessel with activated carbon packing. A residence time of 30 minutes was assumed in order to calculate the volume required. A diameter can then be calculated using a height of 15 meters. The packed height was determined to be 10 meters. This diameter and heights are used to calculate the equipment cost.

Parameters: $Q = 0.05 \text{ m}^3/\text{s}$; residence time = 3 minutes = 1800 seconds; $H = 15 \text{ m}$

$$Volume = 1800 \text{ s} * 0.05 \frac{\text{m}^3}{\text{s}} * 3 = 90 \text{ m}^3$$

$$D = \sqrt{\frac{4*V}{\pi*H}} = \sqrt{\frac{4*90}{\pi*15}} = 2.76 \text{ m}$$

Using EconExpert, total purchased cost = \$106,106.

$$F_{bm}(\text{carbon steel}) = 1.0; F_{mp}(\text{activated carbon}) = 2.5 (\$/\text{kg}) * 480 (\text{kg}/\text{m}^3) / 37550 (\$/\text{m}^3) = 0.32$$

$$C_{\text{carbon packing}} = \$108,284$$

$$C_{BM} = F_{BM} * \$ (106,106 + 108,284) * \left(\frac{595.9}{400}\right) = \$563,027$$

Appendix D: Complete Flowsheet Diagram

Figure D.1. Completed flowsheet with rotary kiln and calciner illustrated.

