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**NAVAL
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MONTEREY, CALIFORNIA

THESIS

**MODELING OF A BUILDING-SCALE LIQUID AIR
ENERGY STORAGE SYSTEM WITH ASPEN HYSYS**

by

Ryan M. Willis

September 2019

Thesis Advisor:

Anthony G. Pollman

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Alejandro S. Hernandez

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**MODELING OF A BUILDING-SCALE LIQUID AIR ENERGY STORAGE
SYSTEM WITH ASPEN HYSYS**

Ryan M. Willis
Lieutenant, United States Navy
BS, Oregon State University, 2012

Submitted in partial fulfillment of the
requirements for the degree of

MASTER OF SCIENCE IN SYSTEMS ENGINEERING

from the

**NAVAL POSTGRADUATE SCHOOL
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ABSTRACT

Solar and wind power generation suffer from intermittency. Consequently, renewable-powered microgrids require a traditional electrical grid or an energy storage system to fill the power gaps. Liquid air energy storage (LAES) is a promising method for scalable energy storage. LAES systems combine three mature technologies—cryogenics, expansion turbines, and induction power generation—into a system of systems. The resultant behavior of this complex system is difficult to predict through analysis alone. Aspen HYSYS, an industrial process modeling and simulation package, was used to create a model of a building-scale cryogenic system based upon a Linde-Hampson cycle. Steady-state cryogenic operations were simulated and model output was validated against a theoretical fundamental comparison. This validated model was then used to implement a parametric, model-based systems engineering approach to design a LAES system for integration into a renewable-powered microgrid at the Naval Postgraduate School's turbo-propulsion lab to counter intermittency. This work is part of a larger effort to evaluate the efficacy of potential energy storage solutions for naval facilities or forward operating bases.

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LIST OF ACRONYMS AND ABBREVIATIONS

ASD(OEPP)	Assistant Secretary of Defense for Operational Energy Plans and Programs
CAES	compressed air energy storage
DoD	Department of Defense
DON	Department of the Navy
E ² O	Expeditionary Energy Office
ES ²	Energy Security and Sustainability Strategy
FOB	forward operating base
HX	heat exchanger
JT	Joule-Thompson
LAES	liquid air energy storage
LAESS	liquid air energy storage system
MBSE	model based system engineering
MBWR	modified Benedict-Webb-Rubin
MORS	Military Operations Research Society
NASA	National Aeronautics and Space Administration
NIST	National Institute of Standards and Technology
NPS	Naval Postgraduate School
NTV	non-tactical vehicle
ONR	Office of Naval Research
OPNAVINST	Chief of Naval Operations instruction
USN	United States Navy
USMC	United States Marine Corp
SECNAV	Secretary of the Navy
SMAP	software management and assurance program

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EXECUTIVE SUMMARY

The Department of Defense manages a wide portfolio of energy demands ranging from traditional fixed facilities to mobile operators such as naval ships and marine forward operating bases (FOBs). Providing the necessary electrical power to these units has become a new facet of strategy when considering operational cost and operational security.

The U.S. Navy (USN) has identified that for shore based naval facilities, electrical power constitutes of 28% of the operational shore budget. This operational cost is the single largest economic burden upon the shore budget (United States Navy 2018). To manage this challenge the Secretary of the Navy (SECNAV) initiated the Navy Shore Energy Program to achieve energy efficiency goals and reductions in energy consumption from non-renewable sources (Office of the Secretary 2017).

The U.S. Marine Corp (USMC) created the USMC Expeditionary Energy Office (E²O) to “analyze, develop and direct the Marine Corp energy strategy in order to optimize expeditionary capabilities across all warfighting functions” (Marine Corps Expeditionary Energy Office 2011). For USMC FOBs, the daily resupply requirement for traditional fossil fuels to run generators presents a no longer acceptable operational risk.

The Energy Security and Sustainability (ES²) Strategy is similar program established by the U.S. Army. One of goals of the ES² Strategy is to migrate to renewable sources of energy, and the strategy identifies microgrids as an enabling technology needed to integrate these new sources (United States Army 2015).

One of the obstacles to the integration of renewable energy sources into islanded microgrids is their characteristic of intermittency. Liquid Air Energy Storage (LAES) is a potential solution to mitigate renewable energy intermittency on islanded microgrids. Renewable microgrid generation in excess of the immediate load runs a cryogenic cycle to create and store liquid air. Liquefied air can subsequently be exposed to ambient heat and expanded through a turbine to recover the stored energy. Using analytic methods to design a LAES and expansion system is complex and time consuming, suggesting modeling and simulation as a preferred approach. Aspen HYSYS, an industrial process modeling

software package, was used to model a combined Linde-Hampson cryogenic cycle (for liquefaction of nitrogen) and an expansion cycle (to convert the energy from liquid nitrogen vaporization to mechanical energy). This modeling approach allows a model based systems engineering approach (MBSE) to the development of a building scale LAES and expansion system.

The first part of this study included validation of the cryogenic cycle using liquid yield as the metric for determining the software model accurately approximated the functioning of an ideal system. Analytical solutions as to the liquid yield were developed by Howe, Pollman and Gannon (2018a) and Barron (1985) and were used as the metric for the fundamental comparison to the software model. Working fluids used in the models included pure oxygen, pure nitrogen, and air (80% nitrogen and 20% oxygen). Two modeling packages applied to the model were modified Benedict-Webb-Rubin (MBWR) and Peng-Robinson. Modified Benedict-Webb-Rubin is a 32-term equation of state package that was more accurate for modeling pure material streams, but is not able to be applied to mixed streams such as air. Peng-Robinson is also an equation of state fluid package and was found to be acceptable for mixed streams such as air.

After validating the performance of the cryogenic cycle, the expansion cycle was added to the model and overall efficiency of the system was used to evaluate the model approximation to an ideal system. The analytical solutions developed by Howe, Pollman and Gannon (2018b) were the metric for comparison. Overall system performance approximated an ideal system accurately only when the number of stages of compression (utilized in the cryogenic cycle) and the stage of expansion (utilized in the expansion cycle) increased. This as expected since the software is intended to model real world behavior, and to have it approximate isothermal compression and expansion required the use of multiple stages.

Aspen HYSYS was validated as an accurate software to model a LAES and expansion system. This will allow a future systems engineer to utilize the developed model to continue the MBSE approach to realizing a functioning system. Utilizing software future work in exploring the system trade space and optimizing operational conditions can be performed in a much more efficient manner.

The thesis presents these findings in the form of two conference papers. The first, “Preliminary Modeling of a Building Scale Liquid Air Energy Storage System with Aspen HYSYS” was presented at the 86th Military Operations Research Society (MORS) Conference in Monterey, California, in June of 2018. The second, “Modeling of a Building Scale Liquid Air Energy Storage and Expansion System with Aspen HYSYS” was presented at the 3rd International Conference on DC Microgrids in Matsue, Japan, in May of 2019.

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I. INTRODUCTION

A. MOTIVATION

The United States Department of Defense (DoD) is a unique organization when considering energy production and storage. The facilities managed by the DoD include traditional brick and mortar installations combined with a variety of forward deployed units. Providing electrical power to a varied portfolio of units in the face of a changing energy production landscape has become a priority for several departments of the DoD.

Motivating much of the change is the development and accessibility of technologies for harnessing distributed resources, along with an increased understanding of the negative impacts of continued reliance on legacy fossil fuels energy systems. With DoD facilities and combatants deployed around the world, the ability to harness local distributed energy sources provides a tangible strategic and economic benefit.

B. MILITARY INVOLVEMENT

The DoD directs an energy policy focused on enhancing military capabilities, improving energy security and mitigating costs. Part of this guidance includes the diversification and expansion of energy supplies and sources. Alternative and renewable fuel sources are areas of focus expressly identified by the DoD (Department of Defense 2014). The Assistant Secretary of Defense for Operational Energy Plans and Programs (ASD(OEPP)) is tasked with overseeing operational energy research in coordination with the private sector and other governmental organizations to identify and demonstrate energy technologies which will support achievement of DoD energy goals (Department of Defense 2014).

The United States Navy (USN) is a principal department of the DoD with substantial energy concerns and goals. Currently, energy expenses represent the single largest cost for USN installations, consuming 28% of the Navy's shore budget (United States Navy 2018a). The desire to reduce this large economic burden and recognition that energy security was a strategic imperative led to the creation of the Navy Shore Energy Program in 2012, under the direction of the Secretary of the Navy (SECNAV) as put forth

by the Department of the Navy Energy Program (Office of the Secretary 2017). The program established goals for energy security:

- Achieve a 30 percent facility energy intensity reduction by 2015.
- Reduce consumption of fossil fuel and increase the use of alternative fuels by the Navy's non-tactical vehicle (NTV) fleet.
- Increase water efficiency of shore infrastructure.
- Reduce greenhouse gas emissions.
- Produce, procure and consume renewable energy.
- Complete annual, comprehensive energy and water evaluations for approximately 25 percent of covered facilities.
- Install, to the maximum extent possible, advanced metering devices on shore facilities that measure electricity, natural gas and steam consumption.
- Promote sustainable development for all new footprint and major recapitalization projects ashore (Office of the Chief of Naval Operations 2012, 2–3).

These defined guiding principles serve the larger energy goals outlined by the SECNAV. To meet the goals of the Navy Shore Energy Program, the Department of the Navy (DON) mandated four concrete requirements:

- Fifty percent ashore consumption reduction by 2020.
- Fifty percent total ashore energy from alternative sources by 2020.
- Fifty percent of installations net-zero consumers by 2020.
- Fifty percent reduction in petroleum used in the commercial fleet by 2015 (Office of the Chief of Naval Operations 2012, 3).

The United States Marine Corp (USMC) is also scrutinizing its own energy culture and the affect it is having on strategic capabilities. Energy requirements for USMC forward operating bases (FOBs) have been growing, reaching a demand of 303 MW requiring 200,000 gallons of fuel per day to support operations in Afghanistan in 2011. To support this large demand, the USMC must supply FOBs with continual logistical support in the form of convoys. These convoys represent a vulnerable target and divert combat power to provide security. During a three month-period in Afghanistan, the USMC was averaging one Marine casualty per every 50 convoys (Pollman 2013).

This identified vulnerability led to the creation of the USMC Expeditionary Energy Office (E²O) with the mission to “analyze, develop, and direct the Marine Corps’ energy strategy in order to optimize expeditionary capabilities across all warfighting functions” (Marine Corps Expeditionary Energy Office 2011). In 2006 then Lieutenant General James Mattis, now Secretary of Defense, said it was necessary to “unleash us from the tether of fuel” (Marine Corps Expeditionary Energy Office 2011). This institutional culture change has brought technologies to the forefront meant to shift dependence from fossil to distributed renewables.

The Army has also established a program to facilitate the move to new energy technologies. The Energy Security and Sustainability (ES²) Strategy is similar to the programs of the USN and USMC in that it lays out an approach to solve energy dependence issues by focusing on increasing efficiency and migrating to distributed renewable energy sources. As well as the energy sources themselves, the ES² strategy identifies microgrids as necessary to integrate a portfolio of newer technologies into a single energy production, storage and distribution system (United States Army 2015).

C. MICROGRIDS

Microgrids are a technology that enables the different DoD departments to integrate new distributed renewable energy sources into forward deployed and traditional home based infrastructures. Chowdury, Chowdurry and Crossley (2009) define a microgrid as a small-scale supply network designed to support the production, storage and distribution of electrical or heat energy to a small community. They identify microgrid technology as

having been applied to industrial parks, universities, housing estates and suburban localities.

A scalable microgrid would facilitate integration of new technologies into the many operational roles required by the DoD. A microgrid designed to support a large naval facility or FOB deployed in the Middle East allows for connection to suitable energy producers consistent with DoD energy goals and enhances operational reach. Figure 1 illustrates how small microgrid would integrate renewable power resources to ensure operation of critical services on an army base.

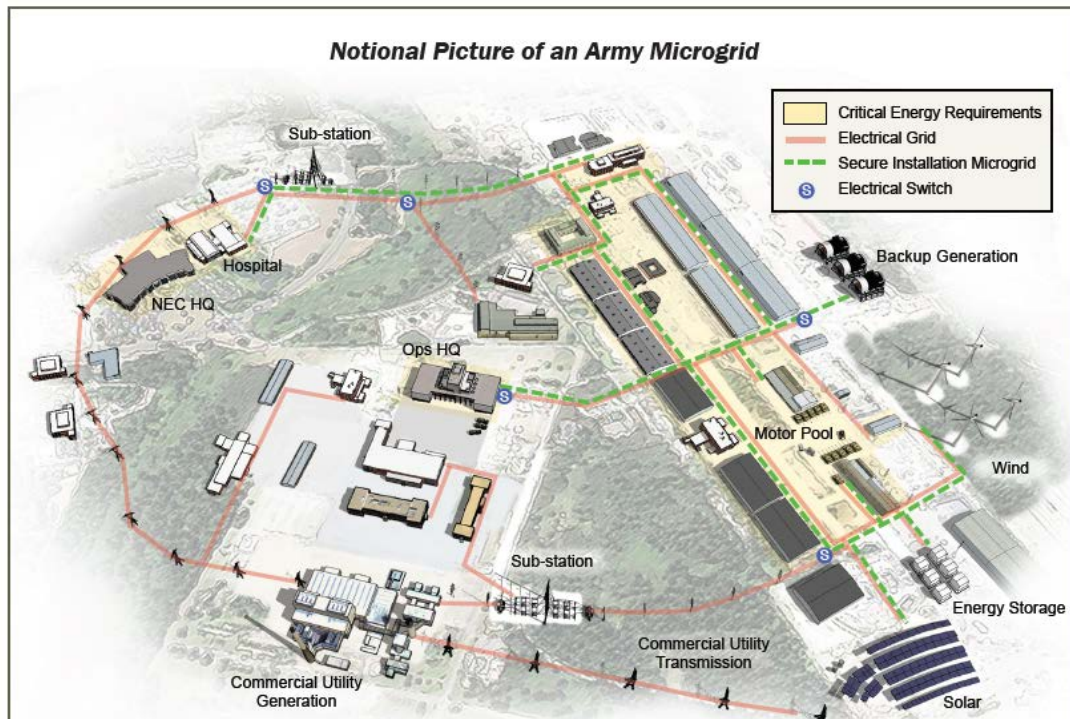


Figure 1. Notional Picture of an Army Microgrid. Source: United States Army (2015).

D. LIQUID AIR ENERGY STORAGE AND EXPANSION SYSTEM

One of the impediments of quickly adopting and integrating distributed renewable energy source is the problem of intermittency. Solar and wind energy are dependent upon fluctuating environmental conditions. To overcome intermittency, excess energy from distributed renewable source require a storage mechanism to access the excess when needed. Batteries, compressed air, liquid air and pumped hydro are all currently available methods to store energy for later use. Diesel fuel is used currently but this dependency upon fossil fuels, even as a back-up system, runs counter to the DoD energy goals.

Some of these options require geographical features in order to be viable. Traditional compressed air energy storage (CAES) systems of adequate size require large storage vessels, usually in the form of underground caverns (McLarnon and Cairns 1989). A site for pumped hydro requires at least two sizeable reservoirs connected to allow movement of water. Geographical limitations such as these make CAES and pumped hydro poor choices for mobile FOBs already constructed.

Liquid air systems present a viable option for excess energy storage. Liquefied air requires less storage volume than that of compressed air for the same potential energy capacity (Wang et al. 2014). While liquid air is considered a newer technology in comparison to the others, it utilizes mature technology that has been employed by the liquid natural gas industry since the 1960s (Castillo and Dorao 2013). Distributed renewable energy sources provide the power to drive a cryogenic cycle to liquefy a vapor, and when these energy sources fall below a needed support threshold, vaporization of the liquefied vapor and the resultant expansion is used to drive a turbine for electrical power generation. The operation of the specific operational principle and system design used in this analysis is discussed later.

E. THESIS OVERVIEW AND SYSTEMS ENGINEERING APPROACH

This thesis uses the conference paper option of using two papers submitted for publication as part of an approved engineering conference. Chapters II and III present the two papers submitted to two different conferences. Chapter II is the article submitted to

and presented at the 86th Military Operations Research Society (MORS) Symposium. Chapter III is the article presented at the 3rd International Conference on DC Microgrids.

This thesis aims to support a model-based systems engineering approach to design and construct a building-scale LAES and expansion system for electrical power generation through a software model. This software model would fall in the first part of the V-Model of systems engineering for defining system requirements. The V-Model, first developed by the National Aeronautics and Space Administration (NASA) for the Software Management and Assurance Program (SMAP), is the chosen model for this analysis (Forsberg and Mooz 1992). A validated software model allows exploration of the system trade space without the need to build and test multiple prototypes. In scaling and designing prototypes, the operation of the constructed prototype can be validated against expected performance as detailed by the software prototype. Figure 2 illustrates the V-Model and where the analysis performed in this thesis falls within the model as applied to the construction of a building-scale LAES and expansion system.

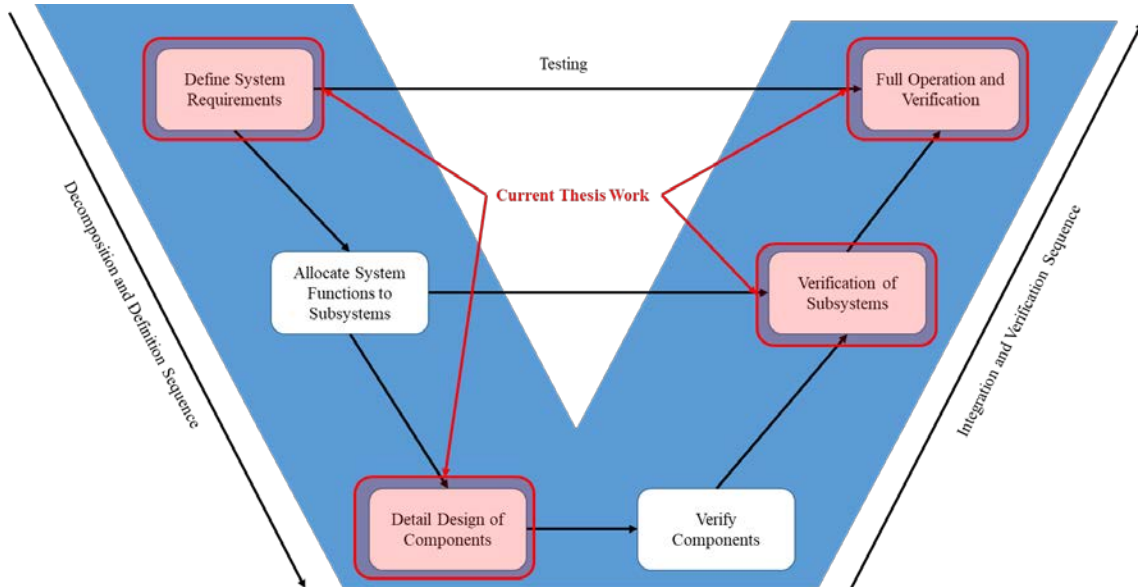


Figure 2. V-Model Identifying Application of Thesis Work in the Development of a Building-Scale LAES and Expansion System. Adapted from Blanchard and Fabrycky (2011).

The software model itself is also a system that must be verified against system requirements. Aspen HYSYS is the chosen software for the development of the model and details to its operation are described in the following chapters. Previous work with Aspen HYSYS for modeling simple Linde-Hampson cryogenic cycles has already been performed. But, none of the previous studies ever validated the results against an accepted standard.

This thesis utilizes previous work from Howe, Pollman and Gannon in 2018 as an acceptable standard for validating the model's proper operation, and therefore, its appropriateness for designing a prototype LAES and expansion system.

The first paper presents a model of the cryogenic phase of the LAES and expansion system. A simple Linde-Hampson cycle is modeled in which after compression of a working fluid, in this case nitrogen, is expanded through a Joule Thompson valve causing liquefaction. Howe, Pollman and Gannon (2018a) performed a closed-form thermodynamic calculation of the Linde-Hampson cycle and developed an expected yield of liquefied nitrogen. Howe compared his results with those obtained by Joshi and Patel (2015). The software model was compared to both previous analytical results to verify proper operation and validate the software as an acceptable tool for analyzing the cryogenic cycle.

In the second paper, the entire LAES and expansion system is modeled. The yield is again validated against previous theoretical solutions. The final validation is a quantitative and qualitative approach with the efficiency of the entire system as the fundamental comparison. Howe, Pollman and Gannon (2018b) produced a study detailing the efficiency of the entire system utilizing an energy and exergy analysis of air.

Chapter IV contains the conclusion as to the validity of the software model as an appropriate tool for the design of a LAES and expansion system. Future work is identified as to the application of the software in the continuing model-based system engineering approach.

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II. PRELIMINARY MODELING OF A BUILDING-SCALE LIQUID AIR ENERGY STORAGE SYSTEM WITH ASPEN HYSYS

This chapter was previously presented as a paper at the Military Operations Research Society Symposium (Willis et al 2018).

CONFERENCE PAPER ABSTRACT

Solar- and wind-power generation suffer from intermittency. Consequently, renewable-powered microgrids often use a traditional electrical grid or an energy storage system to fill the power gaps. Liquid air energy storage (LAES) is a promising method for scalable energy storage. Liquid air energy storage systems (LAESS) combine three mature technologies: cryogenics, expansion turbines, and induction power generation into a system of systems. The resultant behavior of this complex system is difficult to predict through traditional analysis alone. Aspen HYSYS, an industrial process modeling and simulation package, was used to create a model of a building-scale cryogenic system based on a Linde-Hampson cycle. Steady-state cryogenic operations were simulated and model output was validated against a theory-based fundamental comparison. This basic model will be expanded to include power generation. The updated model will then be used to implement a parametric, model-based systems engineering approach to design a LAES system for integration into the renewable-powered microgrid at the Naval Postgraduate School's (NPS) turbo-propulsion lab to counter intermittency. This work is part of a larger effort to evaluate the efficacy of potential energy storage solutions for naval facilities or forward operating bases (FOBs).

A. INTRODUCTION

Energy costs represent the single largest funding expenditure for Navy Installations, consuming approximately 28% of the naval shore budget (United States Navy 2018a). This makes minimizing shore-based energy consumption and investigating energy alternatives a priority (United States Navy 2018b). An aggressive shore energy management program has been pursued since 2010, which resulted in the creation of the Navy's "Shore Energy" program in 2012.

The Shore Energy program as established by OPNAVINST 4100.5E outlined a range of energy goals::

- Achieve a 30 percent facility energy intensity reduction by 2015.
- Reduce greenhouse gas emissions.
- Produce, procure and consume renewable energy.
- Promote sustainable development for all new footprint and major recapitalization projects.
- Achieve fifty percent ashore consumption reduction by 2020.
- Achieve fifty percent total ashore energy from alternative sources by 2020.
- Achieve fifty percent of installations at net-zero consumers by 2020. (Office of the Chief of Naval Operations 2012, 2–3)

The Navy is not the only military branch an interest in pursuing expansion of utilizing renewable and distributed energy resources. The United States Marine Corps (USMC) has recognized that its dependence upon fossil fuels presents a no-longer-acceptable strategy risk and limits operational reach (Pollman 2013). In 2009, the USMC Expeditionary Energy Office (E²O) was formed with the directive to “analyze, develop and direct the Marine Corps’ energy strategy in order to optimize expeditionary capabilities across all warfighting functions” (Marine Corps Expeditionary Energy Office 2011). The USMC continues to explore alternative options to provide power for forward operating bases (FOBs) and other deployed forces (Marine Corps Expeditionary Energy Office 2011).

The Office of Naval Research (ONR), in an effort to explore the feasibility of LAESS, commissioned construction of two small-scale prototypes. Naval Facilities Command Engineering (NAVFAC) constructed one prototype and Nitro-Turbodyne, Inc. was contracted to construct a second (Nitro-Turbodyne, Inc. 2016). Both prototypes were constructed from first principles; however, modeling and simulation were not used to inform the design. Both prototypes failed to yield liquid air. ONR subsequently transferred these prototypes to the NPS for further analysis, re-design, and to support future demonstrations.

B. LAESS DESCRIPTION

A complete LAESS storage system consists of two stages. The cryogenic phase compresses and cools air to liquefaction, and the evaporation phase exposes the liquid to higher temperatures to vaporize the liquid to turn a power turbine.

Figure 3 is a schematic representation of a LAESS in which a simple Linde-Hampson cycle cryogenic system and a pre-cooled Linde-Hampson cryogenic system are used in the initial liquefaction system. In a simple Linde-Hampson cycle makeup and return air at state 1 is compressed to state 2, and is passed to HX-1 where it is cooled to state 3. The Joule-Thompson (JT) valve allows expansion, causing a wet vapor to form at state 4. The liquid reservoir holds liquid air while any gas is recycled and returned to state 1. In the precooled system, HX-1' utilizes a separate external system to cool the gas stream prior to entering HX-1.

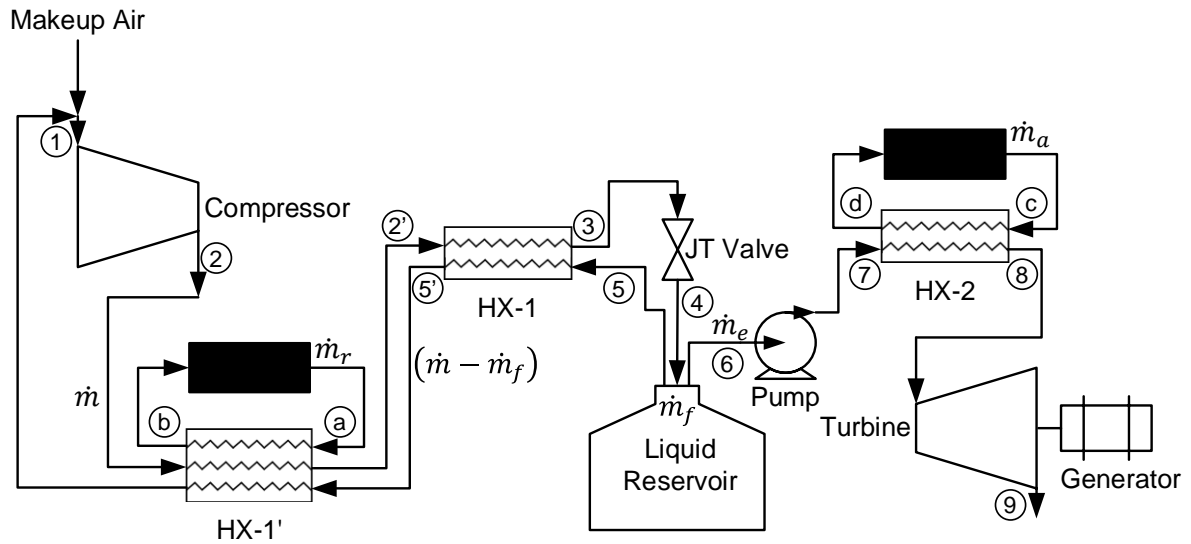


Figure 3. System Diagram of a Liquid Air Energy Storage System.
Source: Howe, Pollman and Gannon (2018b).

On the expansion side a pump moves liquid air to HX-2 where the stream is heated to either ambient or higher temperatures. A turbine utilizes the expansion of this vapor to turn a generator to generate electrical power. The current work is focused on modeling a simple Linde-Hampson cycle, while the expansion stage will be presented in a future paper.

C. MODELING SOFTWARE

Aspen HYSYS is a process-modeling software utilized in the petroleum and chemical industries with a focus on asset optimization. Aspen HYSYS is only one component of a suite of an engineering software offered by AspenTech. The entire Aspen Engineering Suite (AES) allows for many compatible programs to be used to design and optimize complex process models. HYSYS is an artifact-based software, rather than one that utilizes lines of code. The three artifacts utilized are material streams, energy streams and components. Prior to constructing a simulation, components and fluid packages must be selected. Components are those elements and compounds (such as air, nitrogen, oxygen, complex hydrocarbons) that will be utilized in material streams. Fluid packages are the calculation methods utilized by the simulation. Care must be taken in selecting a fluid package that is compatible with the components utilized and the conditions in which the model will be placed (pressure and temperature). One is able to select fluid packages dependent upon the chosen element loaded into the material stream, but would be inaccurate if they applied outside of the pressure and temperature conditions the fluid package was applicable to. Energy streams define energy exchanges within and external to the system (heat in, heat out, work, etc.). Components model real world technology (such as heat exchangers, valves, separators).

Aspen HYSYS was chosen for this examination because previous modeling has been successfully created to examine the Lind-Hampson cycle. In 2015, Joshi and Patel utilized Aspen HYSYS to examine a simple Linde-Hampson cycle. The study utilized a material stream consisting of air with a temperature of 300 K at the system inlet. A compressor with a compression ratio of 320:1 was utilized. Their simulation utilized the MBWR simulation package (Joshi and Patel 2015). Their modeling study of a simple Linde-Hampson cycle was a proof of concept for utilizing the Aspen HYSYS software, but it did not validate the model against any other work. As such, their results were not compared to theory to verify if the model accurately simulated the correct behavior.

D. FUNDAMENTAL COMPARISON

A traditional analysis of a simple Linde-Hampson cycle can be performed utilizing an energy balance with two control volumes: the first containing the compressor and the second encompassing the heat exchanger, JT valve, and the liquid reservoir. Some assumptions must be made prior to conducting the calculations: this is an ideal system which suffers from no leakage and all heat transfer processes are 100% efficient. This also means that the operations performed by the components are ideal. The compressor compresses the gas isothermally, while the JT valve expands the gas in an isentropic process (Barron 1985). Figure 4 is an illustration of a simplified Linde-Hampson system.

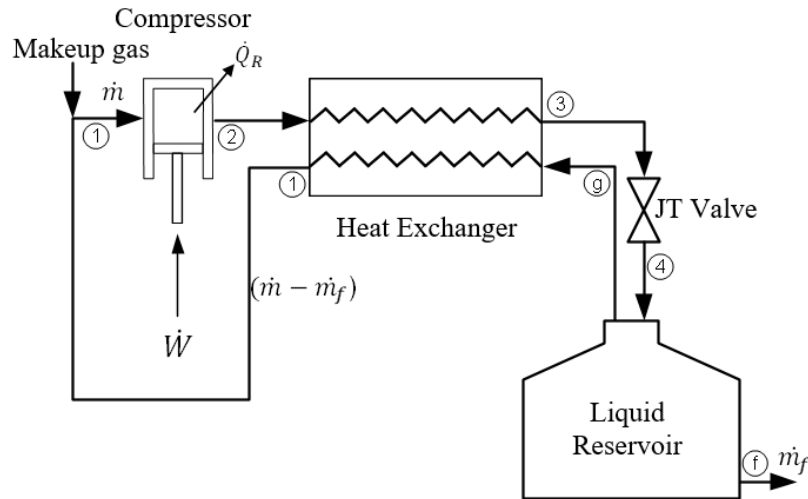


Figure 4. Simplified Linde-Hampson System. Adapted from Barron (1985).

For the sake of this examination the liquid yield (Y) of the system is the fundamental comparison that will be used to validate the proposed model against previous analytical solutions, the fundamental comparison being the results achieved by the traditional analysis and the simulation which allows for direct comparison and validation of the underlying work of each method. The second control volume as described above results in no work or heat being passed into or out of the control volume. This results in a

simple conservation of energy as dictated by the first law of thermodynamics (Barron 1985).

$$\dot{m}h_2 = \dot{m}_f h_f + (\dot{m} - \dot{m}_f)h_1 \quad (1)$$

To obtain the yield, the ratio of liquid mass flow rate to the initial flow rate is solved for (Barron 1985).

$$Y = \frac{\dot{m}_f}{\dot{m}} = \frac{h_2 - h_1}{h_f - h_1} \quad (2)$$

This method was used by both Barron (1985) and repeated by Howe (2018a) on nitrogen, oxygen and air in a Linde-Hampson cycle referencing thermophysical properties of fluids tables. The key differences between these two examinations is Howe utilized newer updated tables from the National Institute of Standards and Technology (NIST), a smaller step size and expanded upon the traditional technique to obtain a novel closed-form solution.

E. CURRENT HYSYS MODEL OF LINDE-HAMPSON

Figure 5 is a depiction of our Aspen HYSYS model. The model was utilized to examine materials streams of pure oxygen, pure nitrogen and air. The air component prebuilt into the software consisted of 80% nitrogen and 20% oxygen. The simulation was performed utilizing two different fluid packages for the sake of comparison: modified Benedict-Webb-Rubin (MBWR) and Peng-Robinson.

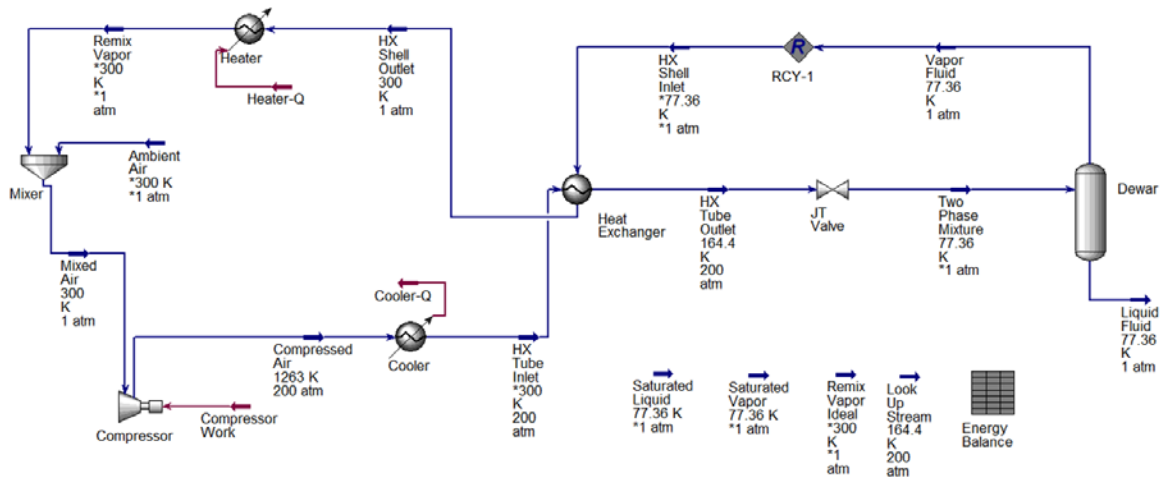


Figure 5. Aspen HYSYS Model of Linde-Hampson Cryogenic System

The MBWR fluid package is a 32-term equation of state that can be utilized for a limited number of pure components that fall within certain temperature and pressure ranges for each component. The result being that only pure oxygen or pure nitrogen could be run through the simulation. It is not possible to utilize the MBWR fluid package with air loaded into the simulation (Aspentech n.d.). But, this is the fluid package that was utilized by Joshi and Patel (2015), and thus it has a proven record of being used to model Linde-Hampson cycles.

Peng-Robinson is another equation of state fluid package which is popular in the natural gas industry (Adewumi n.d.). It is highly useful for hydrocarbon systems with mixed material streams. This allows for pure components (nitrogen and oxygen), as well as mixed material streams (air) to be loaded into simulation (Aspentech n.d.).

The functions of each component of the model are as follows:

- Mixer: Combines the recycled vapor returned from the dewar via the heat exchanger with makeup air from ambient.
- Compressor: Compresses the mixed air stream with a compression ratio of 200:1. This ratio is equal to that utilized by Barron and Howe in previous analytical evaluations.

- Cooler: When used sequentially with the compressor, approximates isothermal compression by cooling the material stream back to ambient temperature.
- Heat Exchanger: An ideal heat exchanger that cools the material stream using recycled vapor from the dewar with zero pressure drop.
- JT Valve: Isentropically expands the material stream resulting in condensing of some of the material stream to liquid resulting in a two-phase mixture.
- Dewar: A separator that divides the vapor and liquid components of the two-phase mixture material stream.
- RCY-1: Recycle function that balances mass equation differences that result from software calculation rounding remainders.
- Heater: Heats recycled vapor back to ambient to mimic ideal cycle.

The material streams labeled Saturated Liquid, Saturated Vapor, Remix Vapor Ideal and Look Up Stream, along with the table Energy Balance, are used to overcome a limitation of the software in performing calculations in the control volume encompassing the heat exchanger, JT valve and dewar. Aspen HYSYS continuously calculates solutions for the state of a material stream or the action of components based upon previous and proceeding artifacts. For example, the energy taken out by the cooler could be determined by defining the material stream on both sides (temperature, pressure, enthalpy), and the software would calculate the amount of heat energy that would need to be removed by the cooler to satisfy those conditions. Another option would be to define the preceding material stream and assign the amount of energy removed by or the temperature difference across the cooler, thus calculating the state of the proceeding material stream. The software is not capable of defining a control volume, then using the energy balances to determine intermediate steps within the control volume. The Energy Balance table performs the necessary calculations to determine the state of the HX Tube Outlet Stream to converge the steady-state system solution for all parts of the model. The calculation is performed

using the yield to determine the quality (X) in the Two Phase Mixture, and then using the isentropic nature of the JT valve to determine the state conditions necessary to define HX Tube Outlet.

$$X = 1 - Y \quad (3)$$

$$h_{\text{Two Phase Mixture}} = h_{\text{Saturated Liquid}} + X(h_{\text{Saturated Vapor}} - h_{\text{Saturated Liquid}}) \quad (4)$$

$$h_{\text{Two Phase Mixture}} = h_{\text{HX Tube Outlet}} \quad (5)$$

After the Energy Balance table performs these calculations, it exports the values to the Look Up Stream, imports the previously unknown temperature from the Look Up Stream and exports that temperature to HX Tube Outlet, thus converging a steady-state solution for the entire simulation. The table is set up to continuously update the state solution, allowing modifications to be made on components and material streams.

F. RESULTS AND DISCUSSION

The simulation was run with the MBWR fluid package on pure streams of oxygen and nitrogen. The obtained yield was compared to the previous examinations of Barron (1985) and Howe, Pollman and Gannon (2018a), as well as a new analytical solution using the state values obtained from the software. This was done to confirm that the simulation was obtaining a thermodynamic steady-state solution that was consistent; it would allow any rounding or other software mathematical calculation discrepancies to be identified. In all, three analytical solutions were compared to simulation results: Barron utilizing tables from 1985, Howe utilizing current NIST tables, and this examination utilizing the property tables inherent to the software. As stated earlier, air cannot be examined using the MBWR fluid package. In all final solutions, yield is expressed as a percentage of fluid flow converted to liquid state. Percent difference is that deviation from the simulation results for the component and fluid package utilized.

Table 1. Analytical and Simulation Results Adapted from Howe (2018a) and Barron (1985).

	Liquid Yield (%); Percent Difference from Simulation (%)			
	Peng-Robinson Simulation	Peng-Robinson Analytical	Barron Analytical	Howe Analytical
Pure Nitrogen	8.47 % ; -	8.47 % ; 0.03 %	7.08 % ; 19.58 %	7.46 % ; 13.49 %
Pure Oxygen	11.80% ; -	11.87 % ; 0.62 %	10.65 % ; 10.80 %	10.63 % ; 11.01 %
Air	9.29 % ; -	9.29 % ; 0.02 %	8.08 % ; 15.01 %	8.08 % ; 15.01 %
	MBWR Simulation	MBWR Analytical	Barron Analytical	Howe Analytical
Pure Nitrogen	7.50 % ; -	7.51 % ; 0.09 %	7.08 % ; 5.97 %	7.46 % ; 0.58 %
Pure Oxygen	10.84 % ; -	10.84 % ; <0.005%	10.65 % ; 1.78 %	10.63 % ; 1.97 %

The results show that the model simulation produced results consistent with previous analytical examinations of the Linde-Hampson cryogenic cycle utilized to liquefy air and air constituents. Analytical solutions obtained from using Aspen HYSYS's own thermodynamic state tables are also consistent with the results obtained from the steady-state simulation solutions.

The MBWR fluid package is slightly more consistent with the previous examinations but is limited in that the composite material stream air was not able to be simulated. The Peng-Robinson was consistent but not as accurate as the MBWR with previous analytical solutions, though, it did have the advantage of modeling a composite material stream.

Either simulation can be used to predict the ideal behavior of a proposed LAESS. This examination has validated that Aspen HYSYS software can be used in future simulations of expanded or more detailed simulations. This validation is a necessary step before using an expanded model to design and construct a building-scale LAESS demonstration.

G. FUTURE RESEARCH

With Aspen HYSYS being validated as a viable option for modeling LAESS, a more detailed model is to be developed to include the secondary side of the system for vaporizing the stored liquid and utilizing the expansion to drive an air turbine for generation of electricity. Once this model is developed, model-based system engineering can be performed to optimize and scale the system.

The current software model is for a small, proof-of-concept prototype; the size being similar to the previously discussed ONR commissioned prototypes. To satisfy the power needs of a building the model will need to be scaled up in size. To scale the model appropriately the necessary electrical output will need to be identified, as well as the electrical power draw the system itself will require to operate. This required electrical power draw is necessary to determine if distributed resources (such as solar, wind) are capable of supporting a full size LAESS.

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III. MODELING OF A BUILDING-SCALE LIQUID AIR ENERGY STORAGE AND EXPANSION SYSTEM WITH ASPEN HYSYS

This chapter was previously presented as a paper at the 3rd International Conference on DC Microgrids (Willis et al. 2019).

CONFERENCE PAPER ABSTRACT

Liquid Air Energy Storage (LAES) is a potential solution to mitigate renewable energy intermittency on islanded microgrids. Renewable microgrid generation in excess of the immediate load runs a cryogenic cycle to create and store liquid air. LAES systems can be combined with an expansion turbine to recover the stored energy. Using analytic methods to design a LAES and expansion system is complex and time consuming, suggesting modeling and simulation as a more efficient approach. Aspen HYSYS, an industrial process modeling software package, was used to model a combined Linde-Hampson cryogenic cycle (for liquefaction of air) and an expansion cycle (to convert the energy from liquid air vaporization to mechanical energy). The model was validated against previous analytic work. The validated model will be used to implement a model-based systems engineering (MBSE) approach to design an LAES and expansion system to reduce intermittency on an experimental microgrid at the Naval Postgraduate School in Monterey, CA, USA. Data from this facility will be used to further modify and validate the HYSYS model.

A. INTRODUCTION

Increased use of renewable energy sources has created a motivation to explore new energy storage concepts to overcome the inherent intermittency problem. A Liquid Air Energy Storage (LAES) system stores excess renewable energy as liquid air, and then using the expansion of the liquid by flashing to vapor to create electrical energy for use when an energy deficit occurs. The system can maintain a storage of condensed vapor while energy from renewables is sufficient; but transitions to vaporization operations when energy from the renewables falls below a required threshold.

This technology is of particular interest to the United States Department of Defense (DoD) due to the rising cost of providing power to military units in garrison and afield. Two of the largest stakeholders within the U.S. DoD are the United States Navy (USN) and the United States Marine Corp (USMC).

The USN has found that energy is the single largest cost for Naval Installations. The current Naval Installation shore budget dedicates 28% towards energy costs, the result being prioritization of reduction in energy costs and consumption (United States Navy 2018a). The official program to address this issue is the Navy's "Shore Energy" program. Established in 2012, and defined in OPNAVINST 4100.5E it created an aggressive set of goals for energy control including, but not limited to, a reduction in greenhouse gas emissions, a reduction of 50% in energy consumption by 2020 and an achievement of 50% of all energy being supplied by renewables by 2020 (Office of the Chief of Naval Operations 2012).

The USMC has determined that the continued dependence upon fossil fuels is no longer an acceptable strategy, because it presents too much risk and limits operational reach (Pollman 2013). The USMC Expeditionary Energy Office (E²O), created in 2009, maintains an energy strategy in order to increase force effectiveness (Marine Corps Expeditionary Energy Office 2011). Alternative sources of power, such as solar, would reduce dependence on fossil fuels which require constant resupply from convoys to forward operating bases (FOBs). In 2010, these convoys supplied 200,000 gallons of fuel per day in Afghanistan, and the vulnerability of convoys resulted in a rate of one marine being wounded for every 50 convoys (Marine Corps Expeditionary Energy Office 2011).

The Office of Naval Research (ONR) is currently funding exploration of an LAES system for integraion into a building scale microgrid. Initial prototype construction and testing conducted by Naval Facilities Command Engineering (NAVFAC) and Nitro-Turbodyne Inc., resulted in two systems that failed to produce liquefied air (Nitro-Turbodyne, Inc. 2016). Neither prototype design utilized modeling or simulation but instead depended only upon designs guided by first principles. The two prototypes have since been transferred to NPS. The goal is to analyze, redesign, build and test a new functional system.

In order to avoid the same results, a model-based system engineering approach was chosen to support design and construction of a small-scale prototype, with an eventual goal of an operational building-scale prototype. Model-based systems engineering is favorable since it is not feasible to continue to construct multiple prototypes and a validated model can inform the design process to increase the probability of a given prototype operating successfully (Blanchard and Fabrycky 2011). However, validation of the model is necessary to verify its usefulness and accuracy in a model-based systems engineering approach. Previous published analytical solutions provide the comparative basis for model validation in this examination.

B. LAES AND EXPANSION SYSTEM

An LAES and expansion system combines the mature technologies of a cryogenic liquefaction with vaporization and expansion to drive a turbine for electrical power generation. Figure 6 is a schematic of the combined cryogenic and expansion subsystems.

The cryogenic system utilizes a Linde-Hampson cycle that cools a working fluid in a heat exchanger (HX-1) and depressurization through a Joule-Thompson (JT) valve to liquefy vapor. The liquid reservoir stores the liquid and directs fluid, still in vapor form, back towards HX-1 for a regenerative cooling process. When electrical power generation is required, a pump moves the liquefied working fluid to HX-2 to vaporize it, followed by expansion through a turbine to turn a generator rotor.

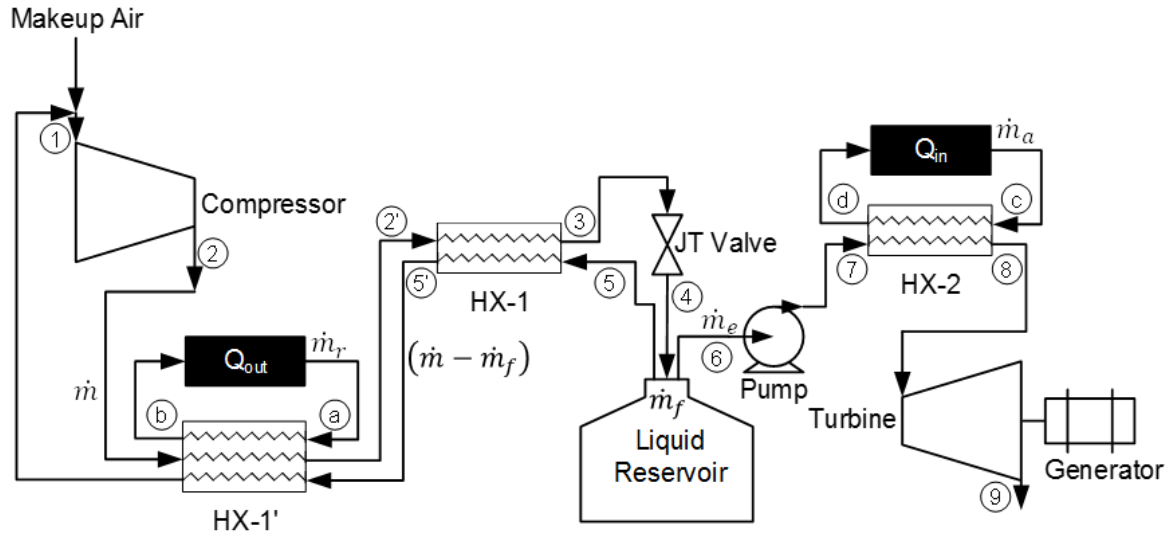


Figure 6. Schematic of a Liquid Air Energy Storage and Expansion System. Source: Howe et al. (2018a).

A second heat exchanger, HX-1', omitted in modeling, is shown in Figure 1 and was included due to previous analytical studies exploring the effects of pre-cooling the working fluid prior to liquefaction. This secondary heat exchanger is not included in this examination because neither current prototype utilizes one and to simplify the modeling process in order to directly identify the conditions that must be achieved in order to obtain liquid air. Later model-based system engineering work will explore the best combination of components and scale to achieve the desired states.

C. MODELING SOFTWARE

As a process modeling software utilized in the petroleum and chemical industries with a focus on asset optimization, Aspen HYSYS is a capable choice for designing a building-scale LAES and expansion system for a building-scale microgrid. Another benefit of the software is its integration into a suite of engineering software for detailed component design. Basic heat exchangers and their boundary conditions can be defined in HYSYS, and then exported to specialized software programs for detailed material and spatial design.

Preliminary modeling and simulation focused on the cryogenic cycle only (Willis et al. 2018). This was done to ensure the software was suitable and accurate before moving to a complete system and because earlier modeling attempts were not validated. Joshi and Patel (2015) modeled a Linde-Hampson cryogenic cycle in Aspen HYSYS but no fundamental comparison to any analytical solution was performed. The work of Howe, Pollman and Bannon (2018a) and Barron (1985) were used as analytical baselines to compare our preliminary model to. The Peng-Robinson fluid package was found to be consistent with theoretical solutions for air to within fifteen percent. The air in the model consists of 80% nitrogen and 20% oxygen. Since future prototypes will utilize air, the Peng-Robinson fluid package was chosen for this work in spite of being less accurate than other fluid packages that are limited to single species analysis (Willis, et al. 2018).

In the preliminary study the percent liquid yield was the fundamental comparison for validating modeling suitability. For the present work, the percent liquid yield was again verified as consistent, to ensure that changes to the simulation to incorporate the expansion phase had not made adverse changes in the cryogenic phase. An output of resulting liquid yields over varying compression ratios was created to compare and validate the full simulation. For the full model, the overall efficiency of the system will be utilized for validation. Howe previously had defined the efficiency as:

$$\eta_{sys} = \frac{\dot{W}_t}{\left(\dot{W}_C/Y\right) + \dot{W}_p + \dot{W}_{HX_1'} + \dot{W}_{HX_2}} \quad (6)$$

Howe (2018a) model an ideal cycle. This equation was modified for this analysis to better fit real system design actions and to be consistent with the inherited prototypes in the hope they can be modified to function properly. Neither prototype featured a precooling heat exchanger (HX-1'). Thus, efficiency for this work was calculated using the equation:

$$\eta_{sys} = \frac{\dot{W}_t}{\dot{W}_C + \dot{W}_p} \quad (7)$$

The coolers in the model outlined in the next section are there to return working fluid streams to equilibrium conditions approximately to ideal conditions. This is needed to create simple stream conditions that can be modified for prototype design and scaling.

The simple software model from previous work was updated to approximate ideal isothermal operations by adding stages of compression and expansion. To achieve this isothermal compression and expansion a cooler or heater was included after a compressor or expansion turbine stage to return the working fluid to isothermal conditions. The pressure ratio for each stage, with n being the number of stages, was calculated by:

$$Pressure\ Ratio = \frac{Outlet\ Pressure}{Inlet\ Pressure} = \sqrt[n]{\frac{Outlet\ Pressure}{Inlet\ Pressure}} \quad (8)$$

D. HYSYS MODEL OF LAES AND EXPANSION SYSTEM

Figure 7 is the software model built in Aspen HYSYS. The working fluid used in simulation is air and the fluid package was Peng-Robinson. Peng-Robinson uses a 26-term equation of state simulation package. These selections are consistent with future plans for a real world prototype as discussed earlier.

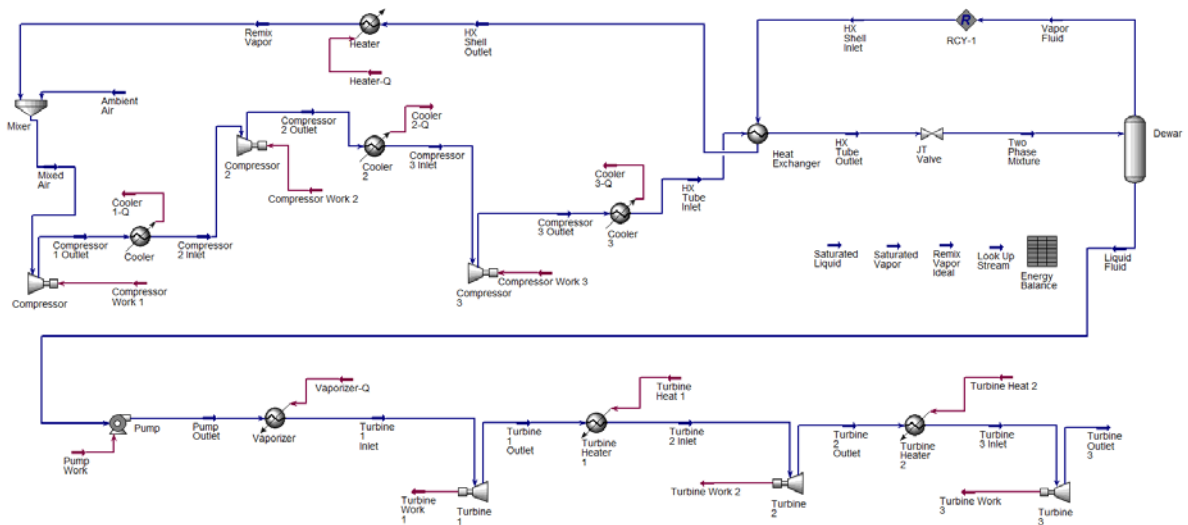


Figure 7. Aspen HYSYS Model of LAES and Expansion System with 3-Stage Compression and Expansion

The functions of each component are as follows

- Mixer: Combines the recycled vapor returned from the dewar via the heat exchanger with makeup air from ambient.
- Compressor: Compresses the mixed air stream. This ratio is equal to that utilized by Barron and Howe in previous analytical evaluations. The compressor has a polytropic efficiency of 100% and an adiabatic efficiency of 99.999%.
- Cooler: Approximates isothermal compression by cooling the material stream back to ambient temperature when used sequentially with the compressor.
- Heat Exchanger: An ideal heat exchanger that cools the material stream using recycled vapor from the dewar with zero pressure drop.
- JT Valve: Isentropically expands the material stream causing condensation of some of the material stream to liquid resulting in a two-phase mixture.
- Dewar: A separator that divides the vapor and fluid components of the two-phase mixture material stream.
- RCY-1: Recycle function that balances mass equation differences that result from software calculation rounding remainders.
- Heater: Heats recycled vapor back to ambient to mimic ideal cycle.
- Pump: Creates pump head to move liquid through expansion cycle. Discharge pressure ratio is 200:1 initially and the pump has an adiabatic efficiency of 100%.
- Vaporizer: Uses heat input to flash liquid nitrogen back to vapor.
- Turbine: Utilizes expansion of air vapor to produce mechanical energy.

- Turbine Heater: Returns material stream to inlet temperature to approximate isothermal expansion.

The Saturated Liquid, Saturated Vapor, Remix Vapor Ideal, Look Up Steam and Energy Balance are needed to overcome software limitations in approximating ideal systems. The pump was included to make the software more useful in later design phases. Currently, the prototype constructed by Nitro-Turbodyne, Inc. uses a check valve operated by differential pressure between the dewar and atmosphere. Since this system was never functionally demonstrated, it was decided to include a pump since most likely future prototypes would require one and to allow study of the trade space in re-pressurizing the air stream prior to expansion. It also allows for validation against previous work done by Howe.

Since this software model is meant to inform design and be verified against a constructed system prototype, the parts and streams were labeled to match real-world corollaries rather than keeping the labeling consistent with Figure 6.

E. RESULTS AND DISCUSSION

Some differences in the output were expected as a result of the modifications made for modeling. Howe, Pollman and Gannon (2018b) utilized isothermal compression in the cryogenic phase while the current work utilized isentropic compression. Isothermal compression in Aspen HYSYS would have to be approximated utilizing a series of compressors with intercooler. The present model approximates isothermal compression and expansion by have a cooler remove added heat from the working fluid post compression and a heater to add heat lost during expansion. This change will result in a lower expected efficiency for the simulation when fewer stages are utilized. The lack of precooling the working fluid prior to compression will also result in a lower efficiency. This is the reason why Howe included it in his energy analysis (Howe, Pollman and Gannon 2018b). The limitations of the software will also result in a reduction in expected efficiency. Aspen HYSYS is an artifact based modeling software for real world systems. This puts some constraints on approximating ideal systems. For example, components do

not function as intended when efficiency is forced to 100%. The expander utilized in the power generation system is set at 99.999% efficiency in order to function.

To verify continued accuracy of the fully developed model, the cryogenic cycle's liquid yield was verified against previous analysis. Figure 8 illustrates the liquid yields obtain by varying State 2 pressure (State 2 is equivalent to HX Tube Inlet in Figure 2). The results are consistent with previous modeling results for yield when utilizing the Peng-Robinson fluid package.

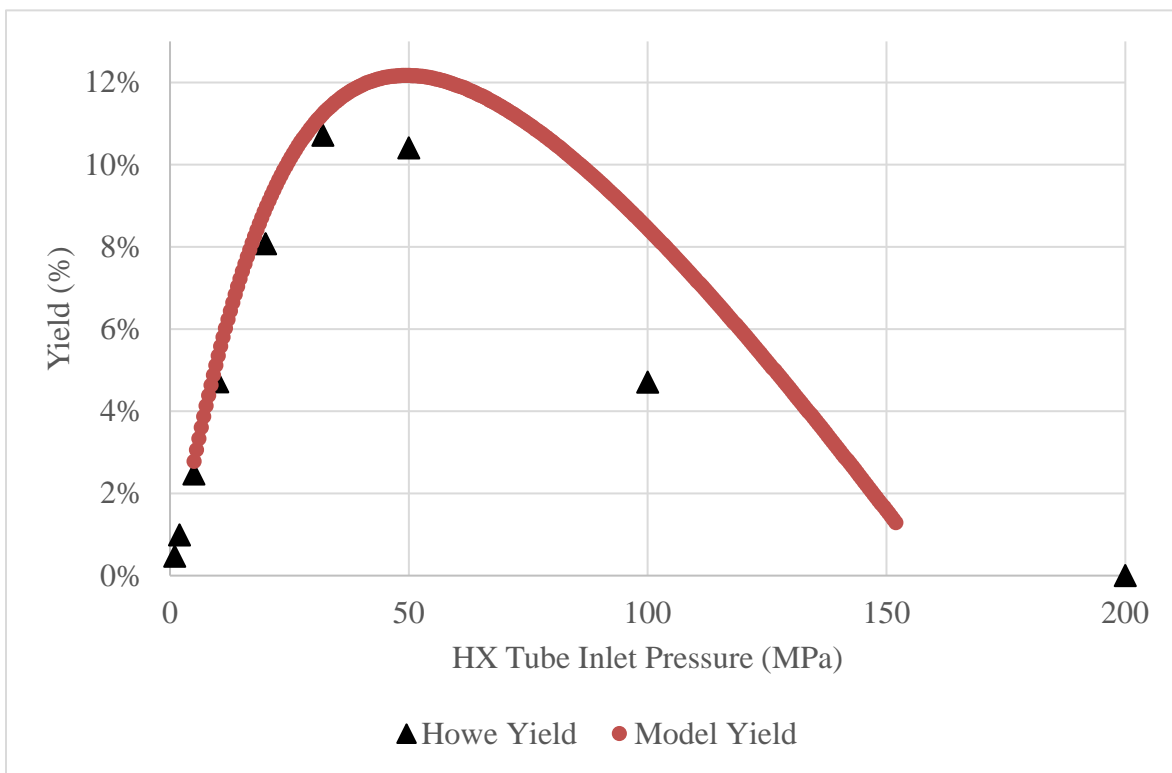


Figure 8. Liquid Yield for Linde-Hampson Subsystem over Varying State 2 Pressures. Adapted from Howe, Pollman and Gannon (2018b).

The difference is explicable due to the difference in working fluid thermodynamic state tables utilized between the different simulations. Howe utilized tables from the National Institute of Standards and Technology (NIST) while this study used those tables intrinsic to the software. Since yields are consistent with previous examinations, this result is acceptable verification for continued model suitability.

The efficiency of the overall system was the final comparison to be used for software model validation. In his previous work, Howe developed performance tables for ideal system using varying pressure combinations for State 2 and State 7 (State 7 is equitable to Pump Outlet in Figure 2). Both the model and Howe utilized air as the working fluid in the efficiency examination. The first model in the present study utilized single stage compression and expansion. This resulted in expected lower efficiencies due to the low fidelity in approximating isothermal compression and expansion. The temperature used in the first model was 300 K for State 2 (State 2 is equivalent to Mixed Air in Figure 7).

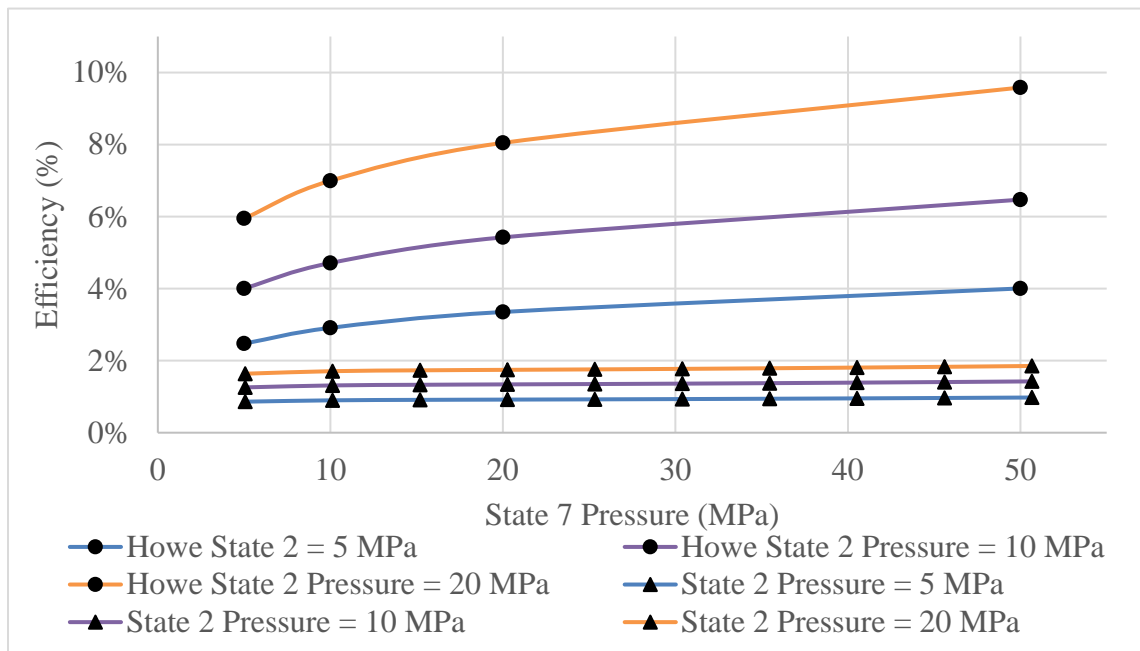


Figure 9. Resulting LAES System Energy Efficiency over Full Range State 7 Pressure and Three Selected State 2' Temperature and State 2' Pressures with 1-Stage Compression and Expansion. Adapted from Howe, Pollman and Gannon (2018b).

An advantage of Howe's ideal examination was the lack limitation on the maximum achievable pressures. Aspen HYSYS has limitations as to the max pressure for which the equations of states can be solved for. These limitations are consistent with those of real world components. Since a direct comparison of all values is limited, a qualitative matching of behavior and values obtained being on the same order of magnitude was considered

acceptable. Figure 10 shows that the efficiency of the system is much lower with only a single compression and expansion phase. The value shown from Figure 10 is that even when varying the operating conditions of the system, the qualitative behavior of the model and theoretical solutions match.

To improve the fidelity of the model and approximate ideal conditions, the number of compression and expansion stages were increased. The pump outlet pressure was varied while the outlet pressure for the compression phase was held constant at 20 MPa.

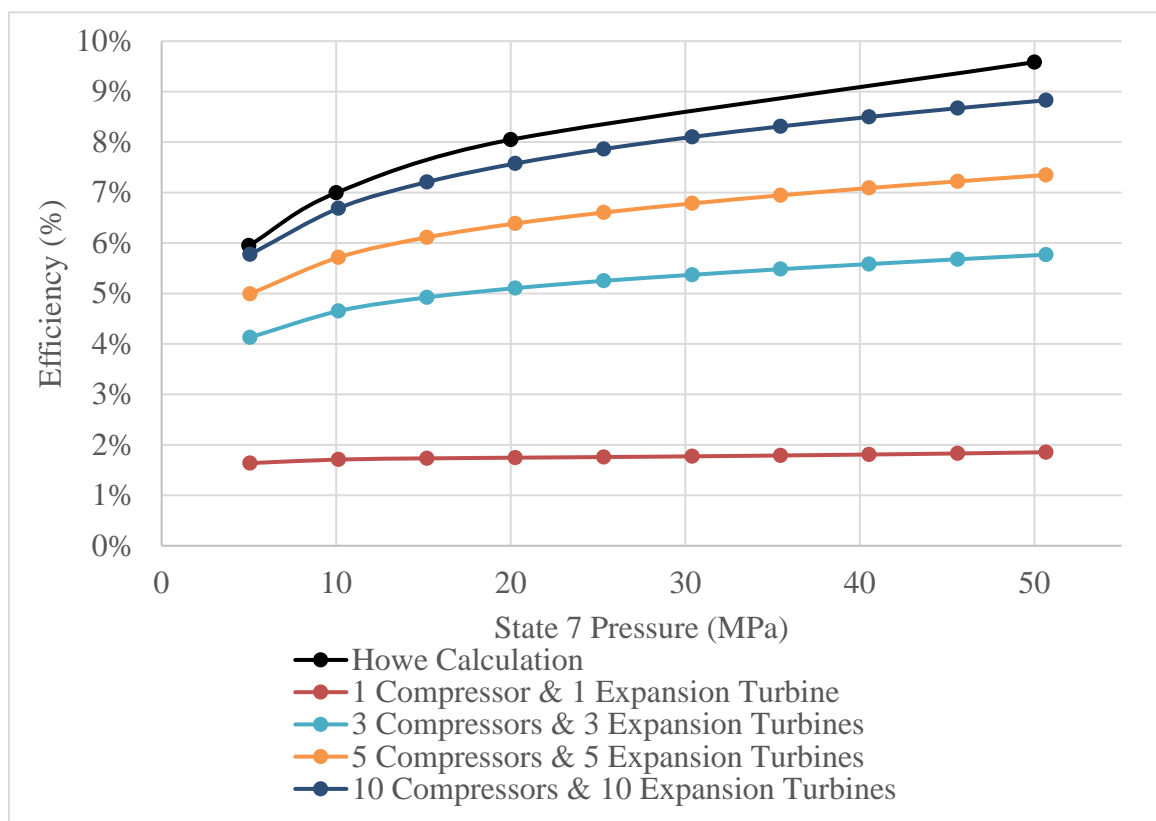


Figure 10. Comparison of Present Work to Previous LAES Storage and Expansion System Efficiencies at 20 MPa State 2' Pressure. Adapted from Howe, Pollman and Gannon (2018b).

Table 2 details the conditions utilized in the modeling with the resultant model efficiency as compared the results obtained by Howe, Pollman and Gannon (2018b).

Table 2. Efficiencies of Theoretical Solution versus Aspen HYSYS Model Efficiency. Adapted from Howe, Pollman and Gannon (2018b).

Number of Stages	Conditions	Howe Efficiency (%)	Model Efficiency (%)
1	State 2 & State 7 Pressure = 20 MPa	8.05	1.75
10	State 2 & State 7 Pressure = 20 MPa	8.05	7.57

Figure 10 illustrates that the overall efficiency of the system increases as the number of compression and expansion stages increase. This is consistent with expected behavior for a model that approximates isothermal process with greater fidelity. As expected the improvement in efficiency for each added stage decreases; the improvement from three to five stages is greater than that from five to ten stages. The model approximates the theoretical solution, and will approach the ideal system as the number of compression and expansion stages approaches infinity.

F. SUMMARY AND FUTURE WORK

A model of an LAES and expansion system was built with Aspen HYSYS, and then used in simulation to produce results that validated the model against analytic results. The model will inform the design and construction of a tabletop prototype. The prototype performance data will then be used to modify the Aspen HYSYS model if necessary.

IV. CONCLUSION AND FUTURE WORK

This thesis presented the motivation and background for the development of a software model of a LAES and expansion system utilizing Aspen HYSYS. A validated software model is vital to an effective model-based systems engineering approach in design.

The first paper outlined the creation of a quantitatively validated software model for the liquefaction phase of a LAES system. A simple Linde-Hampson cycle was utilized and the yield of liquefied nitrogen as compared to that obtained by previous theoretical solutions validated the model as functioning properly. Future performance of an exploration of the trade space for the liquefaction phase can identify ideal operating points and allow for trade off analysis with respect to available commercial-off-the-shelf (COTS) parts. Howe (2018b) identified the heat exchanger as a point of failure in previous LAES system prototypes. With the validated software model, specific performance points and required overall component efficiency can be identified to inform the construction or purchase of an appropriate heat exchanger. This process is applicable to all other components in the LAES system.

The second paper presented a quantitatively and qualitatively validated software model for a complete LAES and expansion system. In agreement with the exergy analysis performed by Howe (2018b) an optimal pressure for air exiting the compressor was identified to be approximately 20 MPa. Future model-based system engineering will again allow exploration of the trade space to scale and optimize a prototype building-scale system.

An LAES and expansion system is a viable option for solving the problem of intermittency when utilizing distributed renewable energy sources to support a microgrid. The validated software model developed in this thesis will be used to execute a model-based systems engineering approach to inform design and explore trade space. As well as identifying system component performance requirements and constraints, the model may be used to identify those environments in which system efficiency and electrical power

generation is maximized. Previous studies have determined that precooling the working fluid prior to compression yielded improved performance. The software model developed in this study utilized ambient temperature for vaporization of liquefied nitrogen. Incorporating precooling and increased vaporization temperatures could lead to identify facilities with existing refrigeration facilities, and excess waste heat available to even further maximize the performance of the system.

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