

# Data-driven Agent Modeling for Liquid Air Energy Storage System with Machine Learning: A Comparative Analysis

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## ABSTRACT

With the wide adoption of renewable energy resources in the power grid, energy storage systems have drawn significant attention to improving the stability and efficiency of the power grid. Among various storage systems, Liquid Air Energy Storage (LAES) has a promising future due to its intrinsic advantages. However, the modeling of a LAES is a complex issue, and existing approaches based on principles have a heavy computational load. To facilitate modeling of LAES, this study focused on data-driven modeling with machine learning and conducted a comparative analysis for several popular methods, including K-Nearest Neighbor (KNN), Support Vector Machine (SVM), Artificial Neural Network (ANN), and Deep Neural Networks (DNN). With LAES as the study case, data-driven models were built based on the data generated by its first-principal model developed with the Aspen HYSYS simulation software. For the selected machine learning methods, the modeling accuracy and running time were compared, showing that the DNN achieved the best performance compared to the others.

**Keywords:** Liquid Air Energy Storage, Machine Learning, Data-driven modeling, Comparative Analysis.

## 1. INTRODUCTION

In the power grid, the demand for electrical energy suffers from significant changes. To meet the dynamic demands of electrical energy on the user side, the conventional approach mainly adjusts the amount of electricity generation such that the generation and energy use are balanced. However, the adoption of renewable energy sources, such as wind and solar

energy, challenges the conventional method for power grid management. Instead, energy storage systems become one of the key approaches to balance the electricity supply and demand in the power grid. At present, large-scale energy storage technologies mainly include battery energy storage, pumped water energy storage, compressed air energy storage, etc. [1].

Battery energy storage systems adopt various batteries (like lithium, lead-acid, or iron-chromium batteries) as energy carriers to exchange electrical energy with the grid. The battery energy storage system has flexible installation and high conversion efficiency, avoiding energy waste. There still lacks a systematic discussion on the construction plan and flexible operation of battery energy storage systems [2]-[4]. Battery systems have the advantages of large capacity, high efficiency, high charge and discharge rate, and long cycle life [5]. However, battery storage systems have higher production costs, limiting their large-scale application to some extent. Contrarily, pumped water energy storage systems are the most cost-effective solutions for large-scale energy storage [6]. Still, they can only be used when the surrounding environment meets the requirements of energy storage power stations. Meanwhile, compressed air energy storage uses surplus electricity when the grid load is low to compress air, and the air is sealed at high pressure in deep underground caves, such as newly built gas storage wells [7], [8]. Several successful large-scale demonstrations of the aforementioned technologies include pumped water energy storage in South Africa and the US, the US isothermal compressed air energy storage system, etc. [9].

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In addition to the mentioned energy storage technologies, Liquid Air Energy Storage (LAES) appears as an innovative and promising technology for large-scale applications in the power grid. It uses a series of compression, cooling, and expansion stages in the Claude refrigeration cycle to liquefy air. The liquid air is stored efficiently in low-pressure, insulated tanks with minimal wastage. Current standalone systems with internal heat integration can achieve 50% and 60% round-trip efficiencies. It is accepted that external supplies of waste heat and cold could increase this substantially to around 70% [10], [11]. The advantages of LAES can be summarized as low initial investment, high energy storage efficiency, flexible adjustment, long operating life, easy maintenance, and is independent of geographic conditions [12]. In [13], a LAES system has been presented in integration with a nuclear power plant.

Despite the advantages of LAES systems, their modeling and real-time operation based on physical principles can be relatively complex and computationally expensive. To tackle this issue, this study investigated data-driven modeling for LAES systems with several most popular machine learning approaches, including K-Nearest Neighbor (KNN), Support Vector Machine (SVM), Artificial Neural Network (ANN), and Deep Neural Networks (DNN). This article uses the methods mentioned above to simulate the LAES process, compares the results of each method, and selects the method with the minor error and relatively best result to replace LAES. The data used in this study are generated from Aspen HYSYS simulation software based on the first-principle model developed for a LAES system. The numerical results demonstrate the advantages of DNN compared to the other approaches according to the comparative effects on modeling accuracy and running time.

## 2. LIQUID AIR ENERGY STORAGE SYSTEM

The energy storage process of Liquid Air simulated by the software is shown in Fig. 1, which can be divided into three parts: compression part, heat exchange part, and expansion part. Air from the environment is compressed in stages and then expanded to ambient pressure and sub-ambient temperature to generate the necessary refrigeration effect to liquefy air. Liquid air is then stored in cryogenic tanks at nearly ambient pressure. During discharge, pressurized liquid air is regasified and expanded through turbomachines to generate electricity and recover stored energy. Both heat of compression and cold thermal energy from regasification can be

stored and recycled to improve the efficiency of the overall system [14].

1) *Compression part*: The compression part in Fig. 1 uses electric energy to drive compressors. First, the air in the environment is purified and compressed before the air is passed into heat exchangers in the heat exchanger part. A gas stream after the separator in the heat exchanger part will be recycled to the compression part.

2) *Heat transfer and storage part*: The heat transfer and storage part in Fig. 1 shows that the pre-cooled air from the compression part is then expanded in a cryogenic expander, resulting in a gas-liquid mixture which is divided into a liquid and a gas stream. The liquid air is stored in cryogenic tanks. The liquid stream is pumped and preheated in evaporators. In this part, the cold energy from liquid air is used to cool air from the compression part.

3) *Expansion part*: The high-pressure air from the heat transfer part is sent to expanders with reheaters. In this way, the stored energy is converted to electricity. Using low-temperature liquid air as an energy storage medium can significantly increase the energy storage density.

As a new large-scale energy storage technology, LAES provides an attractive solution for the efficient and safe use of clean energy. It has the advantages of long life, low pollution, and good compatibility with geological conditions.

Although the LAES is an efficient energy storage solution, the main issue is that its modeling relies on process-based simulation software, such as Aspen HYSYS, leading to complex models and long running time. This causes barriers to the optimization process. For this purpose, the data-driven model is an efficient alternative with specific advantages over process-based simulation.

## 3. MACHINE-LEARNING APPROACHES

### 3.1 K-Nearest Neighbor

The KNN does not require a time-consuming learning process while ensuring moderately good performance [15]. KNN has been widely used in various fields, both for classification and regression. As a classic non-parametric regression model, the KNN algorithm only requires sufficient representative data to model the relationship between input and output. The key idea is to find out the  $k$  nearest neighbors of a sample and assign the average value of some attributes of these neighbors to the sample to get the value of the corresponding attribute. The KNN theory is mature, and the idea is simple and easy to use. However, as the variables gradually increase,

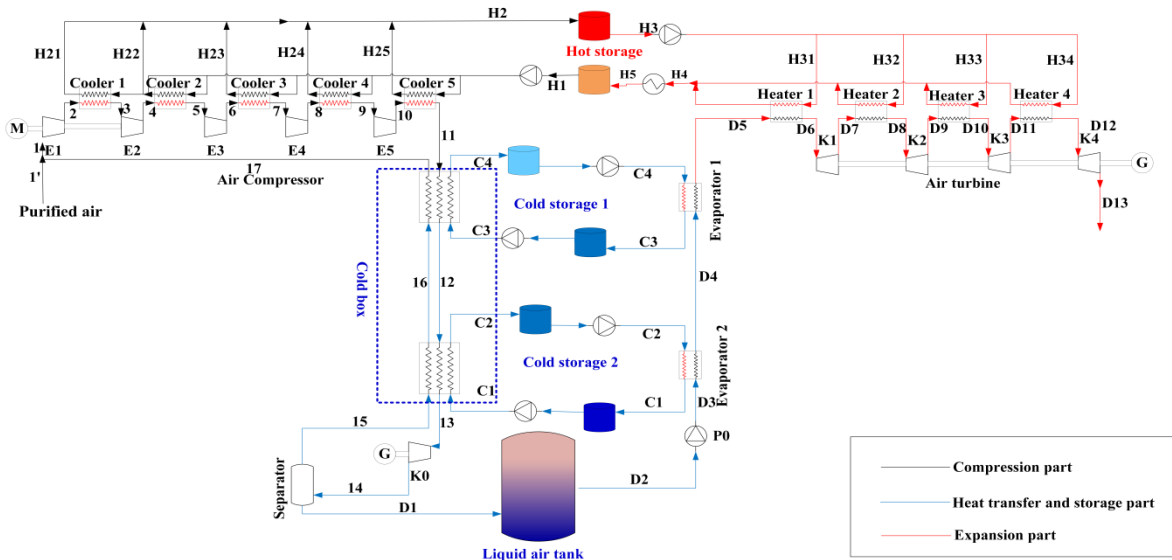


Fig. 1. Schematic diagram of Liquid Air Energy Storage process

the mean value of the variable corresponding to the  $k$  nearest observations may deviate from the actual value of the dependent variable exponentially. When there are many variables, the effect will gradually decrease. Another drawback of KNN is that the calculation speed is slow. The longer the historical data used, the slower the calculation speed becomes, although the accuracy is higher. Overall, KNN is an excellent method that takes advantage of the similarity of historical data.

### 3.2 Support Vector Machine

Support Vector Machine (SVM) is an important branch of machine learning. The essential idea of SVM is to find a hyperplane to separate samples of different categories. The SVM only uses a part of the support vectors to make hyperplane decisions without relying on all data. There are many kernel functions available, which can be very flexible in solving various nonlinear classification regression problems. The SVM method has been used in multiple fields, such as time series forecasting and classification. However, when the data set is huge, it is time-consuming to map the kernel functions of SVM. Assuming a data set  $D = \{(x_1, y_1), (x_2, y_2), (x_3, y_3), \dots, (x_m, y_m)\}$ ,  $y_i \in R$ , the SVM approach can be expressed as:

$$\min_{\omega, b} \frac{1}{2} \|\omega\|^2 + C \sum_{i=1}^m [f(x_i) - y_i] \quad (1a)$$

$$I_{\varepsilon} = \begin{cases} 0, & |f(x) - y| \leq \varepsilon \\ |f(x) - y| - \varepsilon, & |f(x) - y| > \varepsilon \end{cases} \quad (1b)$$

$$f(x) = \omega^T x + b \quad (1c)$$

where  $b$  is the bias vector,  $\omega$  indicates the weight,  $C$  represents the regularization constant,  $\varepsilon$  is the deviation, and  $f(x)$  is the expected regression model.

### 3.3 Artificial Neural Network

Artificial neural network (ANN) is one of the most widely used machine learning methods and achieves excellent performance for huge data set [16]. A neural network is composed of many network units (or neurons) connected. ANN consists of three layers, namely input layer, hidden layer, and output layer, with each layer formed by a number of neurons. The modeling process of ANN is determined by the input and output characteristics of neurons and their connection mode. In ANN, each neuron represents a specific output function, called the activation function. Each connection between two nodes represents a weighted value for the signal passing through the connection, equivalent to the memory of an ANN model. The output of the network varies according to the connection method of the network, the weight value, and the activation function. The network itself is usually an approximation of a certain algorithm, function, or a logical strategy.

### 3.4 Deep Neural Networks

Deep neural network (DNN) is an improvement over ANN with more complex architecture and stronger learning ability. The main difference between DNN over ANN lies in that it has a deeper network depth and trains the network through convolution. Therefore, DNN has stronger non-linear learning and fitting capabilities [17].

For data-driven modeling with DNN, a loss function is required to measure the loss between the output of DNN model and the training sample, as expressed in Eq. (2).

$$J(W, b, x, y) = \frac{1}{2} \|a^L - y\|_2^2 \quad (2)$$

The modeling process with DNN equals minimizing the selected loss function. For DNN, various optimization methods have been proposed, among which the Adam optimization method has become the most popular one [18]. Compared with the traditional gradient descent method, the Adam optimization method dynamically adjusts the learning rate during the learning process and avoids the saddle point problem, difficult to be solved by traditional gradient descent methods [19].

For the loss function  $J(\theta)$ , the general form of the Adam optimization method is expressed in Eqs. (3).

$$cg_t = \nabla_{\theta} J(\theta_{t-1}) \quad (3a)$$

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t \quad (3b)$$

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2 \quad (3c)$$

$$m'_t = m_t / (1 - \beta_1^t) \quad (3d)$$

$$v'_t = v_t / (1 - \beta_2^t) \quad (3e)$$

$$\theta_t = \theta_{t-1} - \frac{\eta}{\sqrt{v'_t + \epsilon}} m'_t \quad (3f)$$

where  $\eta$  is the learning rate,  $g$  refers to the gradient of the current loss function  $J(\theta)$ ,  $m$  and  $v$  are the mean value of the past gradient and the mean value of the gradient square, respectively.  $\beta_1$  and  $\beta_2$  are the set attenuation coefficients,  $\theta$  is the network that needs to be updated parameter,  $t$  is the number of rounds, and  $\epsilon$  is to prevent the denominator from beginning 0.

#### 4. EXPERIMENTAL DESIGN AND ANALYSIS

This section introduces the settings of experiments and analysis of the experimental results. The machine learning methods used in this article were used to model each block of LAES respectively. The outputs of the compression and heat exchange blocks were used as the inputs of the expansion part.

##### 4.1 Setting of Experiments

The data set used in this article is generated from the Aspen Hysys simulation software. The LAES system shown in Fig. 1 is used as the study case, which has been modeled in Aspen HYSYS, to generate data. For the given LAES system, the mass flow 1 is set to 2000 kg/h, and the mass flow 17 is randomly generated in the range of 0 to 500 kg/h with the temperature set to 20 °C. The outputs are obtained through Aspen HYSYS simulation software. After generating the data set, data cleaning has been conducted to filter out all the infeasible items. For the feasible items, 90% were randomly selected as the training set, and the remained items were used to form the test set. With the generated data set, the KNN, SVM, ANN, and DNN methods are firstly used for data-driven modeling based on the training set, after which the

generated models are verified with the test set. In addition, the results based on the test set is compared for various methods on the modeling accuracy and running time.

The settings for machine learning approaches are summarized as the following:

1) For KNN, the value  $k$  is set to 5, indicating that five nearest neighbors are used in the modeling process. This achieved the best performance compared to the values up to 10 for our study case.

2) For SVM, the RBF (Radial Basis Function) is adopted as the kernel function, which is commonly used in nonlinear modeling.

3) For ANN, the number of neurons is set to 8 for the middle layer, which is the value with the best performance compared to the others up to 16.

4) For DNN, the ReLU function is selected as the neuron activation function, the Adam optimization is adopted for the training process, the objective loss function is the mean square error function, and a variable learning rate in the range of 0 to 0.2 is adopted. The number of hidden layers is set to 3 with each layer having 128 neurons and the maximal iteration number is set to 200, which in our case obtains the best performance.

##### 4.2 Experimental results

The modeling error of the power rate for the compression part is given in Fig. 2. It can be found that KNN achieved the best performance for the compressors E1 to E3, while the modeling performance of DNN was significantly improved for the compressors E4 and E5. Since the outputs of E4 and E5 were impacted by the outputs of E1 to E3, the modeling problems had increased complexity and non-linearity, which could be solved better by DNN as described in Section III.

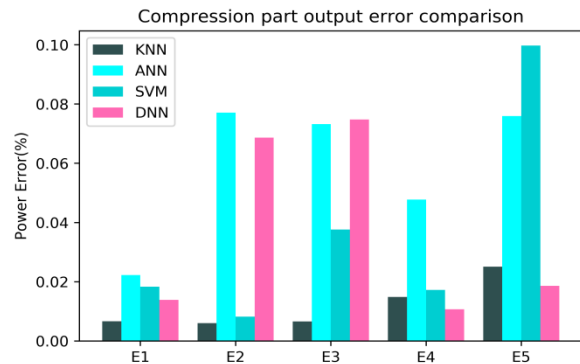


Fig. 2. Modeling error of the power rate in the compressed part.

Figure 3 shows the modeling error of the power rate for the heat transfer and storage part. It can be found that KNN had the least modeling error for P0. On the other hand, ANN achieved the best performance for K0 compared to the others but was not performing well for P0. Further analysis is required to categorize the underlining reasons for the differences.

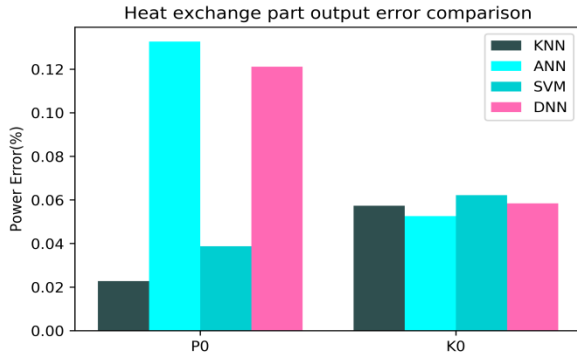


Fig. 3. Modeling error of the power rate in the heat transfer and storage part.

The modeling error of the power rate for the expansion part is shown in Fig. 4. For K1 to K4, the DNN approach outperformed the other three machine learning schemes. However, the KNN method did not perform as well as in the compression part. It is necessary to analyze the causes of this significant difference.

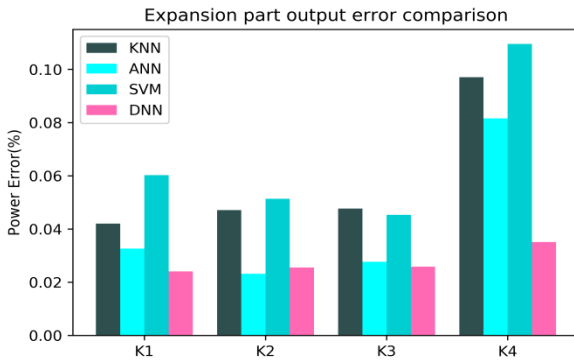


Fig. 4. Modeling error of the power rate in the expansion part.

With the power obtained using various machine learning methods, the round-trip efficiency (RTE) of the entire LAES system is calculated using Eq. (4), in which  $P_x$  indicates the power rate of device  $x$ . The results of RTE are given in Fig. 5. It suggests that the power rate obtained with the DNN approach had the slightest error, much lower than the other three. Meanwhile, it is also worth noting that all the schemes used in this study can model the RTE accurately with an error of less than 5%.

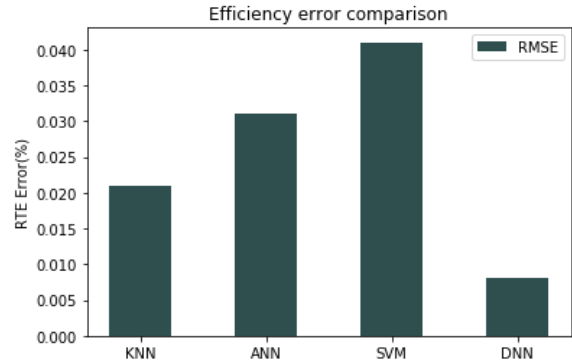


Fig. 5. Error of the integral RTE of the LAES system.

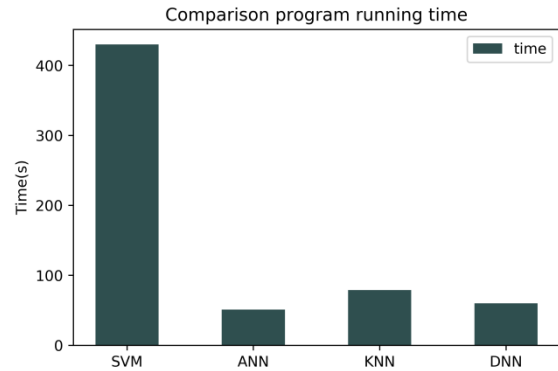


Fig. 6. Running time on the test set.

$$RTE = \frac{P_{E1} + P_{E2} + P_{E3} + P_{E4} + P_{E5} - P_{K0}}{P_{K1} + P_{K2} + P_{K3} + P_{K4} - P_{P0}} \quad (4)$$

In the end, the overall running time on the test set are compared as shown in Fig. 6. Among these four schemes, the SVM had the longest running time greater than 400 seconds, followed by KNN, DNN, and ANN in sequence. It is worth noting that running time between ANN and DNN is negligible while the DNN archived better modeling accuracy.

### 5. CONCLUSION

The wide adoption of renewable energy in the smart grid demands large-scale storage systems to balance the supply-demand relationship. LAES, as a new energy storage technology, has unique advantages for this purpose. In this study, we have conducted a comparative analysis for four commonly used machine learning approaches, including KNN, SVM, ANN, and DNN, to build data-driven models for a given LAES system. Overall, we believe DNN outperforms the other three with the integral consideration of the modeling error of power rate, RTE, and running time on the test set.

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