

Doctoral Dissertation

A Machine Learning Approach to Surrogate Development for Canadian Power System Toward Decarbonization

By:

Zahra Jahangiri

M.Sc., University of Tehran, Tehran, Iran, 2020

B.Sc., University of Tehran, Tehran, Iran, 2016

A Dissertation Submitted in Partial Fulfillment of the Requirements for the Degree of
DOCTOR OF PHILOSOPHY
in the Department of Civil Engineering

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We acknowledge and respect the Lək'wəŋən (Songhees and X'wsepsəm/Esquimalt) Peoples on whose territory the
university stands, and the Lək'wəŋən and W̱SÁNEĆ Peoples whose historical relationships with the land continue to
this day.

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Your love has been my foundation, and I couldn't have done this without you.

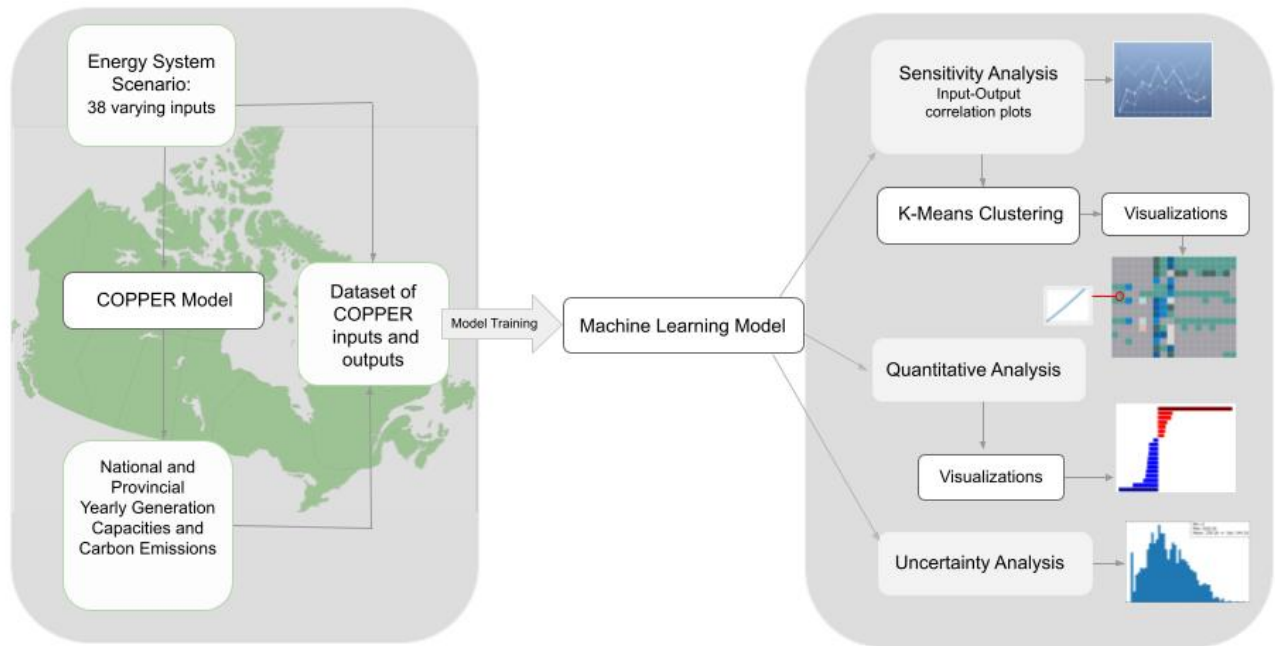
Thank you all for being part of this journey.

Abstract

As Canada works toward a net-zero emissions economy by 2050, understanding optimal strategies for power sector expansion and decarbonization is crucial. To address this challenge, this thesis uses machine learning, specifically neural networks, to conduct a detailed sensitivity analysis, uncertainty analysis and provincial analysis. We developed a supervised learning surrogate model for a capacity expansion model, reducing computation costs by five orders of magnitude. Using this model, we perform sensitivity analysis to evaluate how changes in input variables, such as generation technology capital costs, electricity demand, and carbon taxation, impact model outputs. Additionally, we perform an uncertainty analysis to explore the behavior of the model's outputs in response to variability, uncertainty, and potential fluctuations in these inputs. This approach allows for a more advanced exploration of the design options for Canadian national and provincial power systems.

This model reduces computational time from 11–72 hours to milliseconds with minimal resource requirements. The computational efficiency enables integration into various platforms and tools for decision-making. It's essential because it makes the model accessible to users who may not have technical expertise, such as stakeholders and decision-makers. By reducing the need for extensive technical resources, these users can leverage the model's outputs to inform real-time decisions without relying on advanced computing power.

The study in chapter 4, uses unsupervised machine learning and statistical techniques to identify key factors influencing system outcomes. These include the increasing importance of gas combined cycles in a low-carbon system and the strong potential of wind energy in Canada's decarbonization. Our methodology identifies key patterns in power system outcomes. For example, it uncovers critical correlations like that between variable renewable energy capacity factors and transmission expansion. The results in chapter 5, underscore the importance of flexible grid systems and offering a province-specific roadmap. This thesis introduces the use of machine learning for large-scale energy system planning. It contributes by developing analytical frameworks for model usage and offering a detailed discussion of the results. These insights provide a foundation for strategic planning and policy formulation, particularly in supporting Canada's transition to a sustainable energy future.



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List of publications

This dissertation is written based on the following manuscripts:

- I. Zahra Jahangiri, Mackenzie Judson, Kwang Moo Yi, Madeleine McPherson, “A Deep Learning approach for exploring the design space for the decarbonization of the Canadian electricity system”, *Energies*, “Machine Learning and Data Mining Applications in Power and Multi-Energy Systems” Special Issue, published.
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- III. Zahra Jahangiri, Richard Hendriks, Madeleine McPherson, “A Machine Learning Approach to Analysis of Canadian Provincial Power System Decarbonization”, *Energy Reports*, published.
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In the referenced manuscripts, my contributions include conceptualization, methodology, formulation, design, development of a machine learning-based surrogate model for the large-scale capacity expansion model, extensive scenario exploration using this model, sensitivity and uncertainty analyses, development of an advanced visualization framework, data generation, formal analysis, and writing the original drafts.

Dr. Madeleine McPherson did the original conceptualization of the project by authoring the research grant application. Throughout the thesis process, she provided guidance on all chapters, supervised the work, secured funding, addressed my questions, and reviewed and edited the papers.

Dr. Kwang Moo Yi supervised and addressed all my machine learning inquiries and aided in the conceptualization of the machine learning model. He also provided oversight, supplied resources, and participated in the review and refinement of the written content.

Other researchers contributed to this work as their names appear on the authors for each of the papers. Their contribution to the chapters is covered as follows.

- In chapter three, Mackenzie Judson (PhD student of Civil Engineering at UVic) helped in reviewing and interpretation of the results from a policy planning perspective, as described in the discussion and conclusion sections.
- In chapter four, Mohammad Miri (PhD graduate of Civil Engineering at UVic) assisted in reviewing and interpretation of the results, as presented in the results and discussion sections.
- In chapter five, Richard Henricks (PhD candidate of Civil Engineering at the University of Toronto) contributed to the reviewing, and interpretation of results.

1 Chapter 1: Introduction

Addressing climate change and its impacts has become a major global concern. Decarbonization of the power grid is a critical problem that must be solved to address climate change. However, the path to fully decarbonizing power grids is complex. Understanding the complexities and uncertainties is crucial for developing efficient policies and identifying key opportunities to transform energy systems [3], [4].

Recent studies examined the impact of policies on decarbonization. Jordaan et al. found that provinces with high carbon phase-out and renewable standards reduced emissions. However, the lack of alignment between provincial and federal policies hindered national reductions [11]. A simulation of decarbonization policies showed that carbon pricing alone is not enough. Canada needs additional regulations to limit emissions from natural gas beyond 2030. Inter-provincial transmission development appeared in all least-cost grid decarbonization scenarios [12].

1.1 Canadian Provincial Power System

Electricity services in Canada are regulated provincially. Achieving national emission targets must address provincial differences in economies [13], geographies, technology costs, and policies [14]. Canadian provincial economies differ in their sectoral contributions to gross domestic product (GDP) and in their per capita GDP (Figure 1). Some provinces have abundant renewable, hydroelectric, or nuclear generation with low emissions. However, others rely on fossil fuels, leading to greenhouse gas emissions ranging from 1 to over 670 tCO₂e/GWh [15] (Figure 2).

Each province, despite differences in generation and emissions, follows federal regulations and programs. These include carbon pricing to promote emissions reductions, with an output-based pricing system (OBPS) to protect competitiveness [16], [17], [18]. Federal policies also implement the phase-out of coal-fired generation by 2030 and impose performance standards for natural gas generation at 370 tCO₂e/GWh [19], [20], [21]. Additionally, pending regulations require net-zero provincial electricity systems by 2035 to limit natural gas emissions beyond 2030 [22].

Canadian provinces implement fossil-fuel generation phase-out, renewable portfolio standards, and feed-in-tariffs. While these efforts reduce electricity sector emissions, misaligned federal and provincial policies limit national reductions [11]. Recent studies also indicate that least-cost decarbonization in some provinces entails the development of inter-provincial [23], [24] and international transmission [24], [25]. Multi-year federal efforts aimed at enhancing regional transmission in Atlantic Canada, [26] but provincial utilities opted for a more modest expansion [27].

Figure 1. Canadian provincial differences in per capita GDP C [28], [29]

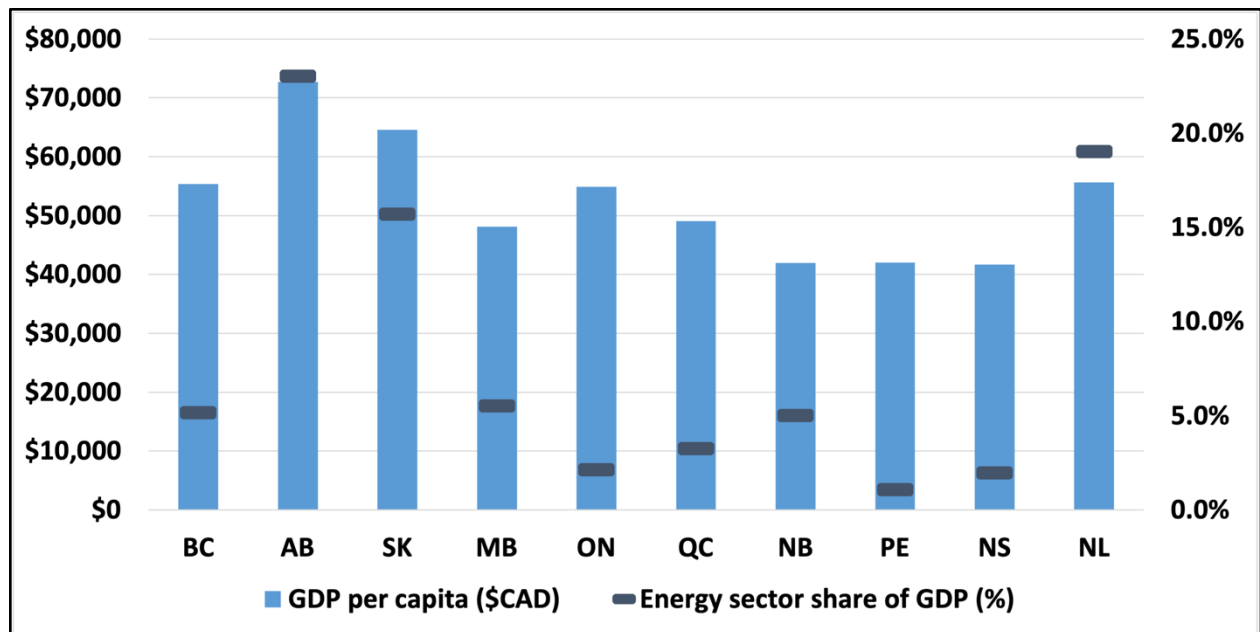
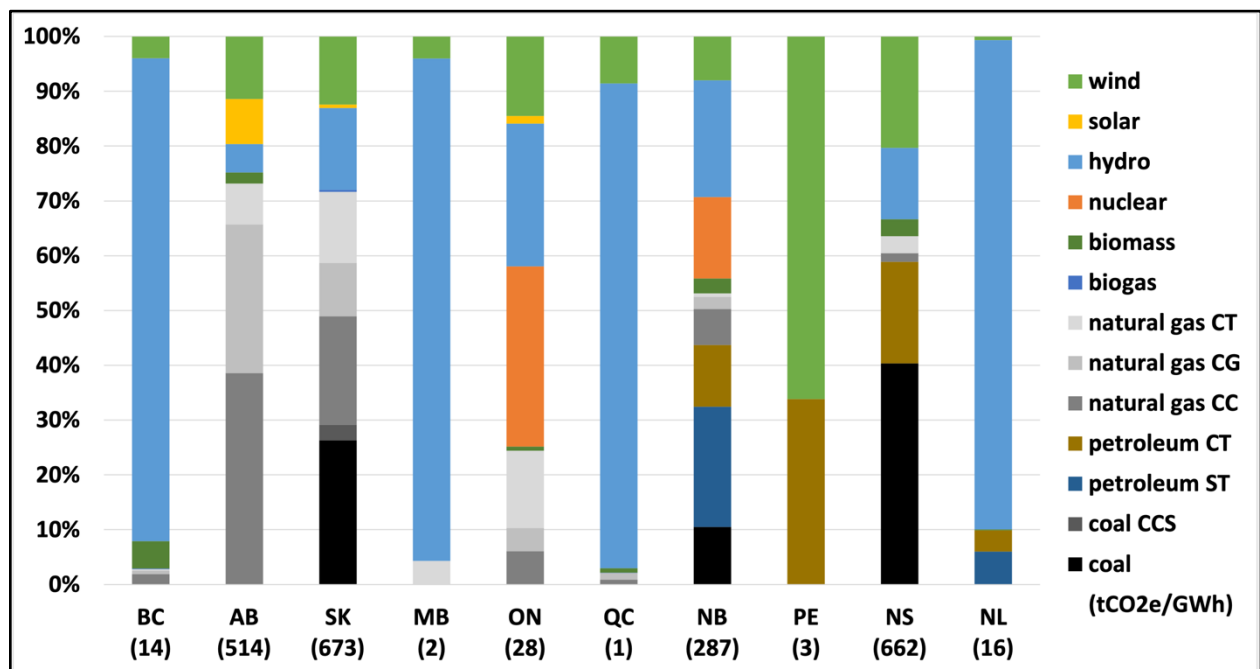


Figure 2. Canadian electricity generation mix and emissions intensities by province



1.1.1 Canadian Policy Context

Renewable Energy development in Ontario is influenced by the legal, policy environment [30], and technology costs [31]. Alberta paused utility board approvals for wind, solar, and hydroelectric projects for seven months to assess environmental impacts, site reclamation, and system reliability [32]. Over 10 GW of Canada's solar capacity is under regulatory review for Alberta's development within four years [33]. This investment likely reflects faster-than-

expected declines in solar capital costs [34]. However, it may also show the unpredictable impact of enabling policies, especially the Alberta Technology Innovation and Emissions Reduction (TIER) Regulation [35]. Introduced in 2018, TIER allows large emitters (>100 kt/y) to meet emissions reductions by lowering facility emissions (e.g., through carbon capture), purchasing performance credits from other facilities, obtaining offset credits from non-obligated facilities, or paying into the TIER Fund.

The NARIS assessment on North American electricity decarbonization found that natural gas generation continued to be developed in the coming decades within the Canadian Western Interconnect (i.e., BC and Alberta) and operated infrequently [24], [36]. A recent NREL study exploring 100% clean electricity options for the US by 2035 found that 21% of dependable capacity came from natural gas turbines. These turbines operated infrequently to meet seasonal peaks, supplying 4% of annual energy [37]. Residual emissions from natural gas generation would need offsets. Costs for non-emitting, flexible generation alternatives remain high. Direct air capture costs are also high due to limited deployment so far [37]. The results of the current study and other deep decarbonization analyses suggest that BC's plan for a 100% Clean Electricity Standard by 2030, which phases out natural gas, should also consider alternative approaches to achieve deep decarbonization [38]. Alternatives could include keeping or building new natural gas generation, with future options for low-carbon fuels, as planned in other provinces [39], [40].

In Canada and elsewhere, policy context is rapidly evolving in response to the electricity system and economy-wide decarbonization needs. The current analysis models to the policy context in place at the time of modelling. In August 2023, the government released the Draft Clean Electricity Regulations. These set a new emissions standard of 30 tCO₂e/GWh. The standard applies to fossil-fueled generation over 25 MW. It takes effect on January 1, 2035, or 20 years after commissioning [41]. Exceptions include peaking units operating up to 450 hours yearly and units with carbon capture technology. These regulations are not yet finalized or included in the Canadian power system model. If adopted, they could significantly change the analysis by adjusting the retirement schedule for fossil-fueled units [12].

Consequently, in the Canadian context, provincial-level analyses are pivotal [42], [43], [15]. They illuminate the unique challenges and characteristics inherent to each province's energy mix, power system, and emissions intensity [44], [11]. This focused approach creates strategies aligned with each province's unique needs. It enables policies that consider resource availability, geography, policy frameworks, and energy requirements across provinces [21], [45].

1.2 Background and Motivation

Recent research shows rising interest in using Machine Learning (ML). ML models aim to overcome the limits of conventional power system modeling [5], [6], [7], [8]. They address the complexity of dynamic, interconnected, evolving power systems [5], [6], [7], [8], [46], [47], [48]. ML, a subset of AI, creates models that enable computers to learn from data and improve performance. ML models can manage complexities and dynamics. This offers potential for improving accuracy and efficiency in power system modeling [46], [49], [9], [10]. These models require

low computing power and resources. Therefore, they offer accessibility and utility for many users. Their efficiency makes them ideal for decision-making platforms, allowing users in various sectors to utilize them without needing extensive expertise or high computing power.

These models' accessibility supports use across industries, from small businesses to government. With a user-friendly interface and low computational requirements, they make advanced analytics accessible for complex scenario analysis. These models efficiently explore extensive scenarios. Users quickly run multiple scenarios to assess outcomes and identify trends or risks. This approach benefits complex decision-making by providing a broad view of possibilities. Users then focus on the most relevant scenarios, where traditional, detailed models can improve accuracy. This two-step approach balances efficiency and precision, enabling broad exploration with detailed insights when needed. Ultimately, integrating these models into decision-making improves forecasting, planning, and strategy. This leads to better-informed decisions and effective outcomes across platforms and tools.[50]

Despite ML advancements in power systems, a gap remains in exploring its potential for large-scale regional or state-level systems, particularly in detecting correlations, uncertainties, and parameter variability.

1.3 Current research status

Current research ML advances renewable energy analysis. It focuses on specific technologies or regions [4]. ML plays a growing role in uncertainty analysis. It improves computational efficiency and accuracy in power systems. However, gaps remain in analyzing systems with many parameters and variables. Current ML efforts focus on optimization and prediction. Exploratory analysis and output space correlations are underexplored.

Research into using Artificial Neural Networks (ANNs) instead of resource-heavy simulations is needed. This shift enables detailed analysis of large-scale power systems. It also supports informed policy and decision-making. Non-linear and path-dependent power system characteristics require tailored analytical methods [4].

Prior research highlights ML's potential to improve power system modeling. However, fully exploring ML's capabilities for regional and large-scale systems remains limited. Understanding and assessing correlations, uncertainties, sustainable policies, and parameter fluctuations is essential. This can enhance efficiency, reliability, and sustainability in power systems.

Addressing these gaps, this research introduces novel surrogate modeling techniques. These methods offer significant improvements and new insights, discussed in the next section.

1.4 The novelty of the proposed research

This thesis explores decarbonizing power systems, ML's role in optimizing power system planning, sensitivity analysis, uncertainty analysis and detailed provincial analysis. It focuses specifically on the Canadian energy landscape at national and provincial levels.

By combining advanced modeling, sensitivity analysis, and provincial insights, it provides actionable knowledge for policymakers, researchers, and industry leaders [51].

The research makes several novel contributions addressing earlier gaps. It takes a multifaceted approach to low-carbon electrification and decarbonization. Three unique elements define this work, detailed further below:

- **Development of ML-based surrogate models for power system planning:** This research introduces and refines ML-based surrogate models for large-scale power system planning. These models enable deeper analysis of the complex dynamics and interactions in large-scale power systems.
The approach outperforms traditional methods by addressing the complexities of evolving power ecosystems. A key goal is to enhance computational efficiency by reducing required time, resources, and model run frequency.
- **Integration of uncertainty analysis for power system planning:** Embedding uncertainty analysis into planning models improves robustness and adaptability. This approach tackles variability and uncertainties in dynamic power systems, supporting resilient and informed decisions.
- **In-Depth provincial analysis of Canadian power system:** This research explores the unique characteristics and variations across provinces. The analysis identifies distinct challenges and opportunities, offering insights into energy mixes, policies, and decarbonization pathways.

This study explores the complexities of power systems to identify pathways and strategies for decarbonizing the Canadian power sector. It incorporates modern advancements, including AI, to ensure innovative power system planning remains up to date.

The approach reduces computational time and resource use in power system modeling, aiming to minimize environmental impact and address global warming. The innovative methods provide critical insights into low-carbon electrification and sustainable energy development. They contribute to ongoing discussions and initiatives.

1.5 Research questions and objectives

This thesis presents ML methods for understanding the Canadian power system. It focuses on decarbonization pathways at national and provincial levels. The goal is to improve sustainable energy planning and decision-making.

Chapter 2 surveys ML techniques in energy systems. It explores how ML improves efficiency, reliability, and sustainability. Different models and architectures are discussed for their energy applications.

Chapter 3 introduces an advanced Electricity System Model using ANNs. This model reduces computational load for capacity expansion analysis. It examines demand growth, carbon pricing, and capital cost variations. Key variables and their sensitivities are identified, and findings are communicated through advanced visualization methods.

Chapter 4 analyzes model output spaces to address non-linear system behaviors. It uses surrogate models to clarify results probabilistically. This approach adjusts multiple inputs to understand system complexities under uncertainty.

Chapter 5 provides a provincial analysis of Canada's power system. It builds surrogate models to capture dynamic changes in provinces. This includes demand growth, cost variations, and policy uncertainties. It explores correlations among factors and aids in adaptable policy development.

Together, these chapters improve efficiency, deepen analysis, and enhance decarbonization understanding. This work supports informed planning and policies for sustainable energy in Canada.

1.6 Thesis structure

The current thesis is structured as below. The second chapter is a review of ML techniques and their application in energy systems, third, fourth, and fifth chapters are manuscripts-based and discuss the introduced research questions accordingly. Each chapter has its literature review, methodology introduction, results, and discussion. In the sixth chapter, a high-level discussion and conclusion are presented. Appendix A includes verification and validation done on the modeling tools that are used in the thesis. Appendix B includes training loss for the model developed in the second chapter. Appendix C lists sources for data and codes that are incorporated in the study.

2 Chapter 2: Review of Machine Learning Techniques and Application in Energy Policy

2.1 Machine Learning Techniques

This section provides a comprehensive survey of ML techniques with the focus on energy systems. The survey covers supervised and unsupervised learning methods, reinforcement learning, and deep learning.

2.1.1 Supervised Learning

Supervised learning train models using labeled datasets with known input-output pairs. The goal is to learn a mapping from inputs to outputs that can generalize to new, unseen data. Operators provide datasets with desired inputs and outputs, while algorithms identify patterns and make predictions. In energy systems, supervised learning is used for demand forecasting, price prediction, and classifying consumption patterns. These models learn from historical data and accurately predict outcomes for new data [52].

2.1.1.1 Regression Models

Regression models predict continuous outcomes based on input features. They are essential for forecasting energy consumption and production [52].

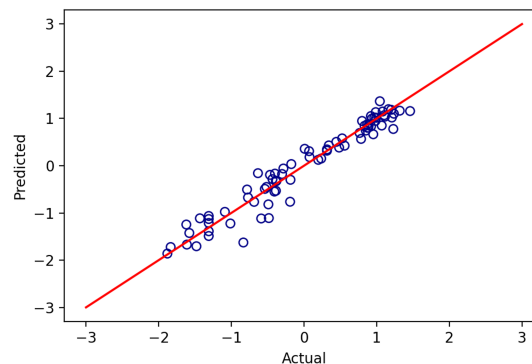


Figure 3 Regression plot show the relationship between the outputs of the model and the actual values of the test data set. The X-axis represents the actual values, while the Y-axis represents the predicted values of the model. The red line ($x=y$) corresponds to the highest level of accuracy, where the predicted and actual values are the same. The closer the blue dots are to the red line, the more accurate the predictions of the model are. These plots allow for visualization of the model's performance.

- Linear Regression: Predicts the output as a linear combination of input features. It's simple and interpretable, making it suitable for initial assessments of energy consumption patterns [52].
- Support Vector Regression (SVR): Captures non-linear relationships by mapping inputs into high-dimensional feature spaces using kernel functions [52].
- Decision Tree: Splits data into subsets based on feature values. It forms a tree structure to predict based on key features [52].

2.1.1.2 Classification Models:

Classification models categorize data into predefined classes. These models are used for categorizing data, such as classifying energy demand into high, medium, and low categories [52].

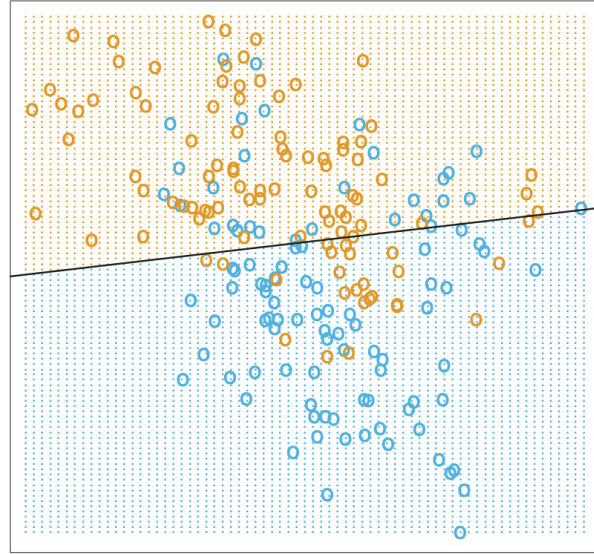


Figure 4 A classification example in two dimensions. The classes are coded as a binary variable (BLUE = 0, ORANGE = 1), and then fit by linear regression. The line is the decision boundary.

- Logistic Regression: Used for binary or multi-class classification problems. It predicts the probability of a class based on input features [52].
- K-Nearest Neighbors (KNN): Classifies data points based on the majority class among the k-nearest neighbors in the feature space [52].
- Random Forests: An ensemble method that uses multiple decision trees to improve classification accuracy by averaging the results of individual trees [52].

2.1.2 Unsupervised Learning

Unsupervised learning uncovers patterns in data without predefined labels. It is useful for exploratory analysis, especially in energy systems. The algorithm identifies correlations and relationships by examining data. It organizes data into clusters or reveals underlying structures [53].

2.1.2.1 Clustering

Clustering groups similar data points together, such as regions with similar energy consumption patterns.

- K-Means Clustering: Partitions data into k clusters based on the mean of the data points.
- Hierarchical Clustering: Builds a hierarchy of clusters using either a bottom-up (agglomerative) or top-down (divisive) approach [54].
- DBSCAN (Density-Based Spatial Clustering of Applications with Noise): Identifies clusters based on the density of data points, making it effective for discovering clusters of varying shapes.

2.1.2.2 Dimensionality Reduction

Dimensionality reduction lowers the number of variables in data. Techniques like PCA and t-SNE reduce data dimensions, enabling easier visualization and interpretation [55].

- Principal Component Analysis (PCA): Transforms data into principal components that capture the most variance [55].
- t-Distributed Stochastic Neighbor Embedding (t-SNE): A non-linear dimensionality reduction technique that preserves local structure. It is ideal for visualizing complex data clusters [56].

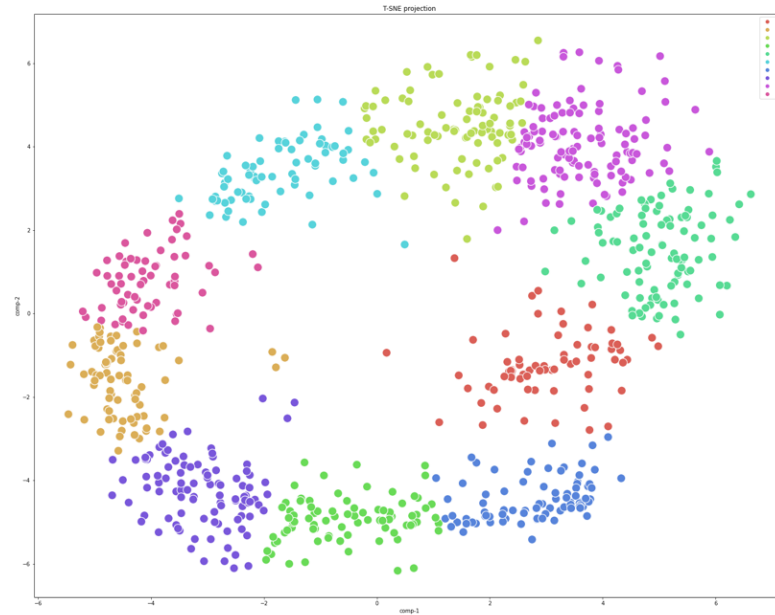


Figure 5 K-means clustering and t-SNE dimensionality reduction to visualize clusters

2.1.3 Semi-Supervised Learning

Semi-supervised learning lies between supervised and unsupervised learning. It leverages both labeled and unlabeled data to improve learning accuracy. It improves accuracy where labeled data is expensive or time-consuming. In energy decarbonization, it is useful for handling large datasets where only a small fraction of the data is labeled. The semi-supervised methods are [57]:

- **Self-training** iteratively trains a model using labeled data. The model predicts on unlabeled data, adding confident predictions to the labeled set for retraining. In energy forecasting, it improves demand predictions by iteratively expanding the training data [57].
- **Co-training** trains multiple classifiers on different data views. Each classifier labels unlabeled data, adding confident predictions to the other's training set. For wind energy forecasting, one classifier uses meteorological (wind speed, temperature) data, another uses geographical (terrain, location) data, iteratively improving through shared labels [57].

- **Graph-based semi-supervised learning** constructs a graph where nodes represent data points, and edges represent similarities between them. Labels are propagated through the graph from labeled to unlabeled nodes based on these similarities [57].
- **Generative models** such as Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs) can be used in semi-supervised settings. They model data distribution to generate new samples. For solar energy prediction, VAEs create synthetic weather data for different conditions to enhance predictive model training [57].

2.1.4 Reinforcement Learning

Reinforcement learning (RL) maximizes cumulative rewards. It uses structured processes to achieve goals. A machine learning (ML) algorithm gets actions, parameters, and outcomes. Within this framework, it explores options and evaluates results. It identifies the best approach by assessing outcomes. RL improves through trial and error. It learns from past actions and adapts to reach optimal results [58]. Two important RL techniques are as follows:

- **Q-Learning:** A model-free RL technique. It evaluates action values in states. Its goal is to maximize rewards.
- **Deep Q-Networks (DQNs):** Combine Q-learning and neural networks. They handle large state-action spaces.

2.1.5 Neural Networks and Deep Learning

Artificial neural networks (ANNs) are among the powerful surrogate models for energy systems [59]. They extract complex insights from a batch of examples (dataset). ANNs replace engineering models for regression, forecasting, and predictions [60], [61].

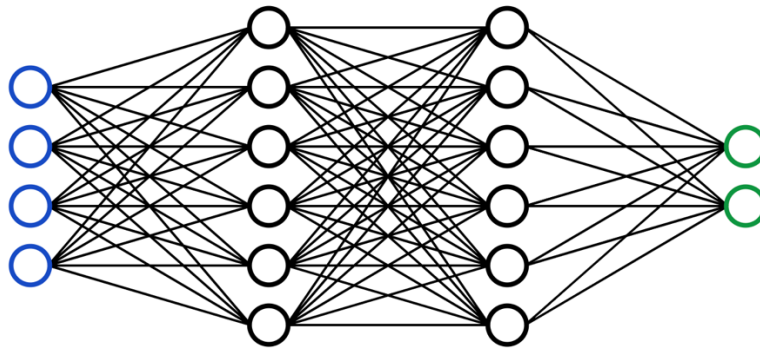


Figure 6 Neural Network Architecture

A neural network (NN) is a function that transforms an input into the desired output. It is a combination of various parameters in multiple layers, to form a function. This function is a nonlinear combination of input features. Thereby, it represents complex mappings precisely. Data is split into training, validation, and test sets. This prevents overfitting and underfitting. The training and validation sets are used for the training process [62].

During training, data is fed to the NN iteratively. The NN adjusts its parameters to minimize the loss function. In regression, loss is the difference between predicted and actual outputs. The model uses the training set to learn from the features of the data to update its parameters. The model repeatedly uses validation to evaluate the performance of the NN. The final model is the one that has the best performance based on the validation set. The ultimate performance of the model is evaluated by a separate independent test set [62], [63].

Adding more layers to a NN makes it deeper. This allows it to extract higher-level features from data. Deep learning (DL) refers to using NNs to model high-level abstractions. DL is a subset of ML involving multi-layered NNs, called "deep" models. These models learn hierarchical data representations. They excel in tasks like image and speech recognition, and time series prediction.

A NN has layers of interconnected nodes (neurons). These nodes process inputs and produce outputs. Each connection has a weight that adjusts during training to reduce errors. Models like Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs) handle complex patterns in energy data. DL handles validation errors differently from traditional regression methods. In DL, the validation error is used as the expected error when feeding new input data. This differs from the usual approach, where validation error is calculated on a separate dataset. Metrics for evaluating deep learning models are low training loss and a small gap between training and validation loss [64]. Deep ANNs extract complex trends in data. But they are prone to overfitting and require longer training times. They also have the risk of vanishing gradients. Adding more layers causes the gradient of the loss function to approach zero. This makes training difficult, a problem known as the vanishing gradient.

Accordingly, we investigate residual connection in residual neural networks (ResNet) [65]. ResNets utilize shortcuts to jump over layers (one or more as shown in Figure 7) with nonlinearities, i.e., activation function, and batch normalization. As shown in Figure 7, $F(x)+x$ simply means that the residual connection adds the value found at the beginning of the block to the end ($F(x)+x$). ResNets are effective in simplifying networks and resolving vanishing gradients [66], [67].

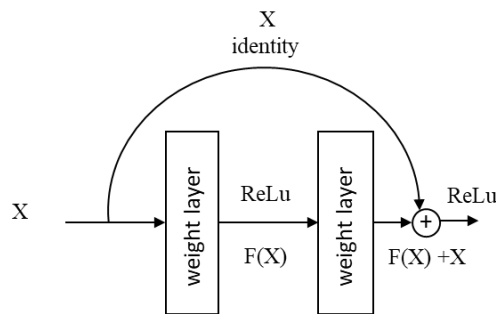


Figure 7 Residual learning: a building block

Below, a short explanation of the main parameters of a neural network is provided:

- Batch size: The number of training examples in one iteration.
- Iteration: One forward and backward pass.

- Epochs: One forward pass and one backward pass of all the training set.
- Learning rate: The step size at each iteration of the optimization process of moving toward a minimum of a loss function.
- Loss function: Mean absolute percentage error.
- Batch normalization: The process of normalizing the layers' inputs in ANNs in order to make them faster and more stable [68].
- Dropouts: Is a regularizer that randomly selects the neurons and ignores them.

More explanation on ANNs and deep learning is provided in the following chapters, as they form the core methodology of this work.

2.2 Applications of ML in the Energy Policy Space

ML can be a transformative tool in the energy policy space. It has the potential to revolutionize how energy systems are analyzed, optimized, and managed. This chapter reviews ML applications in energy policy. It highlights uses, benefits, and challenges. ML analyzes large datasets, predicts trends, optimizes resources, and supports decision-making processes. In this thesis, we categorize ML applications and use cases in energy policy as follows:

2.2.1 Predictive Analytics for Energy Demand and Supply

One of the primary applications of ML in energy policy is predictive analytics. Forecasting energy demand and supply is crucial for policy planning. ML models like time series analysis and deep learning techniques like long short-term memory (LSTM) networks, have been used to predict energy consumption patterns, renewable energy generation, and peak load demands. These predictions help policymakers in optimizing grid operations and planning infrastructure.

Predictive analytics leverages historical and real-time data to identify trends [69]. For instance, ML models can analyze data from smart meters, weather stations, and social media to predict energy consumption in real time. This helps utilities manage supply, reduce costs, and improve reliability [70].

Strielkowski et al. highlight that ML and data-driven methods improve predictive analysis in power systems. They show promise in managing renewable energy variability. The review also notes that these methods effectively handle large data volumes. This capability is critical for future smart grids. However, challenges such as data quality and availability remain obstacles [71].

Khan et al. propose a hybrid ML approach. It combines Multilayer Perceptron (MLP), SVR, and CatBoost for power consumption forecasting. This method integrates trends from renewable and nonrenewable sources. The study highlights the role of accurate energy forecasting in policymaking. It also provides a comparison with other prediction methods [72].

Lin et al. examine China's shift to more renewable energy in power generation. Using ML, they forecast the power mix for the next five years. Their analysis identifies factors influencing this transition. By 2025, thermal power is

projected to make up 60.46% of the mix. Hydropower, nuclear, and non-hydro renewables are expected to account for 20.43%, 6.43%, and 12.68%, respectively [73].

Deng et al. study ML methods for predicting Energy Use Intensity (EUI) in U.S. commercial office buildings. They use data from the 2012 Commercial Building Energy Consumption Survey (CBECS). Their study compares six regression and ML techniques. SVM and Random Forest improve Total EUI prediction accuracy by 10–15% over linear regression. However, linear regression slightly outperforms ML for predicting Plug Loads EUI. The study notes the limitations of the CBECS dataset in predicting energy consumption. It emphasizes the need for more comprehensive data on occupant behavior and building performance [74].

Abualigah et al. review the use of learning-based modeling methods, focusing on DL and ML, for forecasting renewable energy sources such as solar and wind. The study assesses these techniques' performance, highlighting challenges like efficiency, robustness, and accuracy. It emphasizes that learning techniques perform better on large datasets. However, hybrid methods (combining multiple techniques) offer superior accuracy and generalization capabilities. The authors suggest future research on hybrid learning techniques to improve forecasting and optimization [75].

2.2.2 Optimization of Energy Systems

ML algorithms, including RL, are used to optimize energy systems. These optimizations involve load balancing, minimizing energy losses, integrating renewable energy sources, and enhancing the efficiency of energy storage systems [76].

Cao et al. reviewed RL's concepts, algorithms, and power system applications. They highlighted its potential to optimize grid operations and manage distributed energy resources (DERs). RL improves energy efficiency in dynamic conditions. The study also discussed challenges and future directions for RL in energy policy [77].

Alabi et al. review optimization and ML integration in planning Integrated Energy Systems (IES). They emphasize its potential for zero-emission targets and better day-ahead scheduling. The study explores IES structures, modeling, and ML applications. Findings show ML-optimization integration offers benefits but is underexplored in IES. The authors stress the need for an IES framework focused on carbon neutrality. They call for further research to advance ML and optimization integration in this field [78].

Alabi et al. propose a deep reinforcement learning (DRL) agent with automated hyperparameter selection. It optimizes real-time scheduling for a multi-energy system (MES) integrated with CO₂ removal technology (CDRT). Using real-time data from Arizona and CDRT parameters, they evaluate various configurations. The optimized soft-actor critic (SAC) DRL algorithm outperforms the Twin-delayed deep deterministic policy gradient (TD3) algorithm. Results show the DRL agent meets MES and CDRT demands economically, surpassing rule-based scheduling by 23.65%. However, the study concludes CDRT is not viable at current carbon prices. It suggests carbon prices of \$400 – 450/ton and tax incentives could improve viability [79].

Pincioli et al. propose optimizing Operation and Maintenance (O&M) of renewable energy systems using Prognostics & Health Management (PHM) data. This includes health state estimates and Remaining Useful Life (RUL) predictions. They formulate the O&M optimization as a sequential decision problem, solved with DRL. Their solution combines proximal policy optimization and imitation learning for pre-training. Tested on a wind farm scenario and outperforms other DRL algorithms. The approach autonomously discovers the optimal maintenance policy without the need to pre-select a strategy [80].

Yang et al. survey the application of RL in sustainable energy and electric systems. They highlight its ability to handle complexity and uncertainty from integrating intermittent renewables and varying household consumption behaviors. They emphasize that RL, operating without requiring detailed system models, excels in optimizing dynamic systems. The paper reviews the current RL use, discusses growing demand, and outlines future challenges and opportunities to enhance intelligence and flexibility in energy systems [81].

2.2.3 Enhancing Energy Efficiency

ML models are increasingly being utilized to promote energy efficiency across various sectors, including residential, commercial, and industrial. By analyzing consumption patterns and identifying inefficiencies, ML can recommend measures to reduce energy use. Smart grids, equipped with ML algorithms, can dynamically adjust energy distribution to optimize efficiency and reduce waste. Additionally, ML-driven energy management systems can monitor and control energy consumption in real-time, leading to significant cost savings and environmental benefits [82].

In buildings, ML can be used to optimize heating, ventilation, and air conditioning (HVAC) systems, lighting, and other energy-consuming devices. By learning from historical data and real-time inputs, ML models can predict occupancy patterns and adjust energy use, accordingly, leading to substantial energy savings [83].

Pham et al. propose a Random Forests (RF) model for predicting short-term hourly energy consumption in buildings, evaluating its performance using five one-year datasets. The RF model demonstrated high accuracy, with mean absolute error (MAE) values ranging from 0.430 to 0.940 kWh across different prediction horizons. Compared to the M5P and Random Tree (RT) models, the RF model showed superior performance, with improvements of up to 49.21% in MAE and 46.93% in mean absolute percentage error (MAPE) for 1-step-ahead predictions. The study highlights the RF model's effectiveness and its potential as a valuable tool for enhancing energy efficiency in buildings [84].

Zekić-Sušac et al. explore the integration of Big Data and ML into energy management systems for public sector buildings, focusing on smart city applications. They compare prediction models using DNNs, regression trees, and RF, finding that RF provided the highest accuracy. The study proposes an intelligent system, MERIDA, which combines Big Data and predictive models to enhance energy efficiency in Croatian public sector buildings. The paper discusses the technological requirements for developing MERIDA, which aims to support public administration in reducing energy consumption, costs, and improving overall building performance within smart cities [85].

Wang et al. review the practical challenges of implementing ML models for building energy efficiency, focusing on real-world applications rather than just algorithmic performance. The study analyzes existing research on ML in building energy management, identifies issues in implementation, and proposes potential solutions. It covers the model implementation process, practical issues, and future research directions, including technology discovery, data governance, and generalizability testing. The review aims to enhance understanding and guide future research on applying ML for improving building energy efficiency [86].

Tien et al. review the application of ML and DL techniques in the built environment, focusing on their use in optimizing HVAC systems, energy forecasting, indoor air quality, and fault detection. They highlight the challenges in selecting the most suitable AI models due to the diverse range of algorithms, scopes, and evaluation metrics used in existing research. While AI has shown promise in enhancing building performance, most studies remain experimental, with limited implementation and post-occupancy evaluation in real-world buildings. The review calls for more specific guidelines and further development to establish best practices in applying AI to building energy efficiency [87].

2.2.4 Policy Analysis and Design

ML techniques, such as clustering and classification, are instrumental in policy analysis and design. These methods can analyze large datasets to identify trends, segment populations, and predict the impact of various policy scenarios. For example, ML can help assess effects of carbon pricing, subsidies for renewable energy, and regulations on energy consumption. By offering data-driven insights, ML enables the creation of effective and targeted energy policies [88]. Clustering algorithms can group regions or populations based on energy consumption patterns. This enables targeted policy interventions. Classification models can predict the outcomes of different policy scenarios. They can help policymakers choose the most effective strategies for reducing emissions and promote renewable energy.

Arbolino et al. propose a novel approach for ex post monitoring of environmental policies implemented by Italian regions. They use a hierarchical cluster analysis. The study shows significant improvements in policy effectiveness, in Southern regions, between 2008 and 2015. A panel data model offers insights into optimal financial allocation among various renewable energy types. This approach supports pollutant reduction and alignment with European Union energy policies [89].

Csereklyei et al. analyze energy mix evolution in EU member states from 1971 to 2010 using model-based clustering. They identify seven key energy profiles and observe progress towards higher quality energy mixes. However, infrastructure and resources availability create inertia. Higher energy quality correlates with higher income and per capita energy use. The study highlights convergence in energy intensity and links domestic resources to import dependency [90].

Ebers et al. analyzed nearly 500 forest biomass energy policies using a four-tier classification system. They categorized policies by approach, type, subcategory, and specification. The study also uses cluster analysis, showing

that neighboring states often had similar policy profiles. Oregon had the most tax incentives and biomass-specific policies, while Southern and Midwestern states had fewer policies. The study suggests classification and clustering can guide policy development by sharing successful policy approaches across regions [91].

Christensen et al. show that a ML-based predictions of retrofit impacts in building energy efficiency programs are more accurate than traditional engineering models. Their analysis of Illinois's energy efficiency program shows that targeting high-return interventions increases net social benefits. Returns improved from \$0.93 to \$1.23 per dollar invested. This approach addresses the common issue of energy savings falling short of forecasts and improves resource allocation for climate policy [92].

Ahmad et al. propose a Gaussian Process Regression (GPR) model for short/medium-term energy, solar, and wind power forecasts. It addresses the challenges from anomalous weather conditions for energy policy applications. Their study uses four experimental methods with different kernel functions and data resolutions to improve forecast accuracy. The GPR model outperforms existing models, providing reliable predictions across temporal resolutions. This approach enhances planning for energy reliability and productivity during extreme weather events [93].

Perera et al. propose a data-driven approach using RL to design distributed energy systems. This addresses the limitations of traditional white box models in managing complex energy flows and uncertainties. They compare two NN architectures—fully connected and CNN—against a grey box model based on fuzzy logic. The study finds that RL with a fully connected network improves objective function values by 60% compared to the grey box model, while the CNN approach offers an additional 20% improvement. This study shows that data-driven models excel in optimizing complex energy systems, advancing distributed energy system design [94].

The application of ML enhances energy system efficiency and reliability. It supports sustainability by leveraging predictive analytics and optimization. These methods equip policymakers to design and implement effective policies. While challenges in data, algorithms, and computation exist, advancements expand ML's capabilities. As ML evolves, its integration into energy policy becomes essential. It optimizes resource allocation, improves grid operations, and enables sustainable energy solutions.

In this work, NNs and deep learning are chosen over traditional ML methods. They handle high-dimensional, nonlinear, and complex datasets better. NNs learn hierarchical representations, capturing intricate energy system relationships. This includes renewable energy variability and system interdependencies. Deep learning architectures like fully connected and residual networks address scalability issues. They solve challenges like vanishing gradients in deeper models. These models create accurate surrogates for design space exploration. Policymakers use them to evaluate scenarios and improve decisions. Other ML methods, such as clustering and dimensionality reduction, are also employed. They enhance the interpretability of surrogate model results by uncovering patterns and simplifying data. Deep learning supports optimized designs and informed decisions under uncertainty. It provides a robust solution for large-scale energy system modeling.

2.3 Surrogate Modeling and Output-Space Exploration: Methods, Challenges, and Design Decisions

2.3.1 Motivation: Beyond Marginal Uncertainty to Structured Output-Space Insight

The COPPER model encodes a high-dimensional, nonlinear mapping from a set of input levers, carbon tax trajectories, technology costs, demand growth, transmission expansions, and policy constraints, to a rich vector of system-level outputs including generation by technology, emissions, storage deployment, and interprovincial flows. This mapping exhibits sharp regime changes (bifurcations), multimodal outcomes, and complex interdependencies among outputs that are both policy-relevant and non-intuitive. Traditional uncertainty quantification approaches (e.g., Bayesian calibration, simple Monte Carlo sampling of individual outputs, or marginal sensitivity analysis) are insufficient in this context because they either (1) fail to scale to the joint, high-dimensional output space or (2) collapse dependencies by providing only isolated, marginal distributions. What is required for robust planning is not merely “what is the probability of outcome X?” but a structured understanding of *how* outputs co-vary, where pathways diverge, which combinations of uncertainties produce qualitatively distinct futures, and what latent dependencies drive scenario heterogeneity.

To meet this need, we implemented a two-stage methodological pipeline. First, we constructed a fast, accurate surrogate model capable of emulating COPPER’s mapping across the entire input domain, producing thousands of coherent system-level output realizations with negligible computational cost compared to the original optimization runs. Second, we applied a suite of statistical and information-theoretic analyses on the generated output ensemble—mutual information, rank correlations, and clustering—to uncover nonlinear dependencies, system bifurcations, and dominant pathway structures. This decoupling of sample generation from structured interpretation enabled an exploratory uncertainty analysis that reveals both the breadth of plausible futures and the mechanisms by which input uncertainties manifest as output variability. The following subsections document the experimental trajectory: initial surrogate attempts, architectural challenges, design solutions, training protocols, and the rationale for the chosen uncertainty analysis strategy.

2.3.2 Initial Surrogate Attempts: Shallow ANNs and Their Limitations

Our first surrogate modeling experiments used conventional feedforward artificial neural networks (ANNs) with limited depth (one to three hidden layers) and standard nonlinearities (ReLU/tanh). These architectures were trained directly on the input-output pairs generated from Latin Hypercube Sampling (LHS) across the specified uncertainty ranges of COPPER’s inputs. The goal was to learn a direct mapping from uncertain inputs to the bundle of national and provincial outputs for 2030, 2040, and 2050.

While shallow ANNs offered some predictive signal, they consistently underfit critical structures in the output space. Quantitatively, the test set R^2 values were significantly low, and the mean squared error (MSE) residuals displayed structured patterns rather than random noise, indicating systematic mismatch. This loss of modality was especially evident when comparing true output histograms (e.g., for gas SC generation showing clear dual peaks under varying

carbon tax) against surrogate-generated distributions, which were unimodal and lacked the divergence necessary to distinguish the pathways highlighted in later analysis.

These failures exposed two core challenges of the surrogate task: (1) the need to model highly nonlinear, heterogeneous output behavior—some regions of input space induce smooth responses, others induce sharp discontinuities—and (2) the requirement to generalize reliably across both dense and sparsely sampled regions, including extremes that are policy-significant but rare. The inability of shallow ANNs to disentangle these patterns motivated a transition to deeper architectures with enhanced training mechanisms.

2.3.3 Depth Introduced: Challenges with Naïve Deep Networks

Deep neural networks offer greater expressive power through hierarchical composition of nonlinear transformations, which is theoretically well suited to capture the layered dependencies present in the COPPER input-output mapping. However, moving to deeper fully connected MLPs introduced optimization challenges in practice. The two main issues were:

Vanishing/Exploding Gradients: As depths increased beyond a few layers, gradient signal propagation deteriorated, especially in early layers responsible for coarse-grained structure of the mapping. This led to slow convergence, plateaued loss curves, and catastrophic forgetting of simpler input-output relations during training.

Training Instability and Overfitting: Deeper networks became sensitive to initialization and learning rate choices; without architectural mitigation, networks either failed to learn (stagnant loss) or overfit local pockets of the training distribution while degrading in generalization elsewhere.

Empirically, deeper plain MLPs (e.g., 6–8 layers) showed marginal improvement in training loss but inconsistent test performance, particularly in capturing the extremal and multimodal behaviors that were central to downstream pathway analysis. These observations indicated that capacity alone was insufficient; the network required structural modifications to stabilize learning and preserve meaningful gradients across depth.

2.3.4 Residual Architecture Design to Overcome Optimization Barriers

To mitigate the gradient degradation and enable deeper, reliable function approximation, we adopted a **residual neural network** (ResNet) architecture. The central idea of residual learning is to reparameterize each layer (or block) to learn a corrective residual. This identity shortcut connection provides direct signal paths making it easier to learn mappings close to identity and preserves gradient flow during backpropagation, addressing both vanishing gradients and representation flexibility. The block’s input is added to the output of this subnetwork before passing to the next block.

Comparative ablation experiments showed that removing residual connections from otherwise identical deep architectures caused convergence to degrade, and the surrogate’s ability to reproduce multimodal output histograms collapsing. This empirically confirmed the residual design as foundational for the surrogate’s success.

2.3.5 Stabilization & Regularization: Batch Normalization, Dropout, and Architectural Choices

Beyond residual connections, several auxiliary architectural and training mechanisms were incorporated to further stabilize optimization, improve generalization across sparse regions, and control overfitting.

Batch Normalization: Implemented after each linear transformation and before activation within residual branches, batch normalization reduced internal covariate shift, allowing higher effective learning rates and smoothing the loss landscape. Its inclusion resulted in faster convergence and lower sensitivity to initialization variance. Empirically, models with batch normalization showed fewer spurious oscillations in early-loss trajectories.

Dropout: To prevent overfitting—particularly important because the surrogate must extrapolate reasonably in combinations of input variables not densely sampled—were applied selectively. Dropout macro-averaged error on held-out validation folds increased robustness to noise and reduced variance in output predictions across randomized training seeds.

Activation Functions: We experimented with standard ReLU, leaky ReLU, and GELU activations. ReLU offered stable training and was chosen for the final architecture due to its balance of computational simplicity and empirical performance; variants showed marginal benefits in some outputs but introduced training irregularities in others, leading to inconsistent behavior across the heterogeneous output set.

These mechanisms collectively made the deeper residual surrogate tractable to train and able to generalize, supporting the generation of coherent, high-fidelity output samples necessary for downstream analysis.

2.3.6 Hyperparameter Search and Model Selection

To identify configurations that balanced fidelity, robustness, and computational efficiency, an extensive hyperparameter search was conducted over the following axes: number of residual blocks, hidden layer widths, learning rate, batch size, and dropout. The search strategy combined random exploration for broad coverage with targeted grid refinement around promising regions.

2.3.7 Uncertainty Analysis: Limitations of Standard Methods and the Chosen Pipeline

Standard uncertainty quantification techniques in energy systems, such as Bayesian calibration, sampling of individual input parameters, or direct scenario comparison, are typically oriented toward estimating marginal distributions of specific outcomes or require prohibitive computational budgets to probe joint behaviors. They often obscure the structural interdependencies between outputs, cannot readily elucidate regime shifts (e.g., when small changes in carbon tax trigger qualitatively different generation mixes), and fail to give planners a mechanistic map of the output space.

To overcome these limitations, our pipeline uses the trained surrogate to quickly sample a large ensemble of outputs across the input domain. Each surrogate query (i.e., a set of input parameters) yields a coherent vector of provincial and national outputs. By generating thousands of such vectors, we produce a high-resolution empirical approximation of the joint output distribution under input uncertainty. This ensemble becomes the substrate for

structured analysis: rather than asking “what is the probability distribution of X ?” we examine “how do variables interact?”, “which outputs drive divergence?”, and “how do clusters of scenarios group according to dominant behaviors?”

Notably, this approach is not purely predictive; it explicitly separates generation from interpretation. The surrogate is used as a fast mechanism to sweep across the design space, and the downstream statistical machinery interrogates the behavior of that space in ways standard methods cannot: uncovering non-linear dependencies, identifying deterministic “axes” vs. stochastic ones, and revealing latent “pathways” or clusters that correspond to coherent decarbonization trajectories.

These analyses, only feasible at the scale enabled by surrogate sampling, convert the raw uncertainty into interpretable structure. The outputs of these methods feed directly into the insights presented in later chapters—identifying robust technologies, bifurcation conditions, and leverage points that would have been invisible under marginal or low-resolution uncertainty treatments.

3 Chapter 3: A Deep Learning approach for exploring the design space for the decarbonization of the Canadian electricity system

The content of this chapter is published in the following journal:

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3.1 Abstract

Conventional energy system models have limitations in evaluating complex low-carbon transitions and addressing climate change. To address this, we propose a model for exploring a broader design space. We develop a supervised machine learning surrogate of a capacity expansion model using residual neural networks. This surrogate accurately approximates the model’s outputs while reducing computation costs by five orders of magnitude. The increased efficiency allows for sensitivity analysis of outputs to inputs, providing insights into system development factors for the Canadian electricity system from 2030 to 2050. To interpret and communicate surrogate model results, we propose an easy-to-interpret method using unsupervised machine learning. Our analysis identifies and quantifies key factors. Carbon tax and wind energy capital cost are the most impactful factors on emissions in most provinces. They are 2 to 4 times more impactful than other factors on the development of wind and natural gas generation nationally. The model deepens our understanding of the most effective decarbonization policy interventions.

Keywords: *Decision making; Deep learning; Energy decarbonization; Energy planning; K-Means clustering; Machine learning; Power systems; Residual neural networks*

3.2 Introduction

Global greenhouse gas (GHG) emissions must reach net-zero by 2050–2070. This aligns with the Paris climate agreement to limit warming below 2°C. Decarbonizing energy systems can prevent further climate crises [1]. Adoption of new technologies and policies across all sectors can accelerate this transition [2]. The ultimate goal is to shift from fossil fuels to sustainable, low-carbon energy sources.

Decarbonization of the power system is central to the decarbonization of the entire energy system. This is because many fossil fuel displacement technologies are electrified devices that rely on electricity. They will not achieve significant emissions reductions if the electricity they use is generated from high-carbon sources.

3.2.1 Modelling the energy system transition

Energy Systems Models (ESM) are used by researchers and engineering analysts to analyze interrelated technical, socio-economic, and spatiotemporal factors in the energy sector [95]. These models are particularly useful for assessing the viability of energy systems, such as the electricity sector, to meet energy demand [96], [97]. Conventional ESMs for the electricity sector are typically based on established principles in the field, such as power systems engineering and economics. They are used to optimize technically feasible systems for the least-cost. Then,

the decision-makers use the insights gained from these models to explore alternative pathways and design and evaluate policy [98].

Decision-makers require holistic insights to effectively and accurately evaluate system-level policy responses in a timely manner. However, conventional ESMs are limited in their ability to provide holistic analysis. They have high computational load for simulating scenarios of transformative systemic change, such as those needed to achieve GHG targets or climate stabilization. These limitations are further compounded when comparing multiple scenarios, making it difficult to identify high-level interactions within the system for policy planning. For example, ESMs are not able to directly quantify the generalized effect of an input parameter (e.g., price of wind energy) on a target output variable (e.g., carbon emissions). Instead, many scenario runs are needed to search for a trend. Conducting comprehensive sensitivity analyses to assess the robustness of findings is often computationally infeasible.

There is a need to improve ESM methods. This supports Canada's decarbonization obligations by predicting complex relationships. It connects key sectors to the broader socio-economic landscape [5], [99]. Increasing the computational efficiency of ESMs enables the generation of broader, deeper, and more relevant quantifiable insights delivered by modelling a much wider range of scenarios. A computationally efficient ESM:

1. Facilitates the development of robust, well-supported policy options, including identification of the most critical policy-planning inputs.
2. Provides insights into critical energy system design relationships. These insights were inaccessible with conventional ESMs. They change decarbonization discussions and enable large-scale, impact-ranked policy assessments.

We demonstrate that the creation of a novel type of ESM based on surrogate modelling techniques using machine learning (ML) can achieve these goals.

3.2.2 Literature review

When an engineering model is computationally expensive, surrogate modeling can reduce the burden. Surrogate models mimic the behavior of the base model with lower computational costs. An ML-based surrogate is trained on input-output data from the original model and then validated. It predicts outputs for many input sets quickly without requiring extensive resources. This reduction enables broader design space exploration, sensitivity analysis, uncertainty analysis, and optimization [6], [7].

Surrogate models have been deployed in a variety of engineering disciplines, but their use in describing energy systems is a relatively new area with significant potential. Successful implementation of surrogate techniques have been reported in the context of building energy system models [6]; ML techniques are widely used in this field for creating efficient models, reducing computational cost, and providing faster predictions [8].

3.2.2.1 Machine learning for energy systems analysis

ML techniques have been shown to be effective in exploring a wide range of design options and scenarios for energy systems [5]. If the training dataset is well-populated within the input value range, scenarios with any combination

of input parameters can be examined quickly. This requires no specialized resources. Other ML methods such as classification [100], clustering [101], and outlier detection [102] are capable of extracting similarities and outliers, as well as clustering the results and their input features based on the objective of the problem. Classification methods provide the model with the ability to accurately predict the class of a label for unseen instances of data [103]. Clustering methods group unlabeled examples based on their similarities and outlier detection methods identify abnormal data. Examples of these techniques in energy systems include the classification of power quality distribution at power system frequency and out of power system frequency [104], outlier detection for identification of abnormally high or low energy use in a building [105], and automatic identification of operational cycles and patterns within complex building energy system [106].

Studies show ML methods effectively represent energy systems. They require minimal assumptions about historical or synthesized data. ML extracts complex patterns that are hard to explain mathematically from physical principles. Mosavi et al. [5] reviewed publications that have used various supervised learning methods for a wide range of applications in renewable energy systems and planning. Many of the works reviewed confirmed the ability of supervised algorithms, specifically neural networks (NNs), to extract complex features from a batch of examples in the energy systems context. Zhang et al. [107] compared a collection of ML algorithms as surrogate models for electrical and heating networks with the objective of integrating renewables into the Dutch energy system. Their results showed that the linear regression model and the long short-term memory model had the highest performance the best in each electrical and heating network. Sciazko [108] implemented various interpolation techniques and NN architectures to develop surrogate models for a steam energy network. The study resulted in the generalization of features of different types of surrogate models and the use of a surrogate model for optimization with a genetic algorithm. Kim et al. [109] employed NN to predict energy consumption in an actual building's air conditioning system. The model developed in this study enabled forecasting energy consumption with limited variables. The authors reported relatively high accuracy but acknowledged that a sufficient amount of data and model improvement were necessary to achieve even higher accuracy. Uselis et al. [110] studied the use of localized convolutional neural networks for geospatial wind forecasting. They compared the recent state-of-the-art spatiotemporal prediction models on the same data. They concluded that convolutional layers can be extended with localization. Harrison-Atlas et al. [111] used an ML technique, namely boosted regression trees, for spatially-explicit prediction of capacity density advances geographic characterization of wind power potential. The study's findings indicated that this methodology could improve the characterization of spatial aspects of technical potential. This is a critical element in delivering reliable and actionable conclusions from renewable energy scenarios. Antonopoulos et al. [112] conducted a review of the use of artificial intelligence approaches to model energy demand response with the aim of cost-effectively enhancing the flexibility and reliability of energy systems. This review outlines directions for future research in this rapidly growing area by discussing the advantages and potential limitations of artificial intelligence/ML techniques for different demand response tasks. Ahmad and Chen [103] review the ML forecasting growth and their real-time applications in various energy systems. The authors conclude that supervised

learning approaches are suitable for regression problems, like short-term load and price forecasting. NNs also have a wide range of applications in the decarbonization of energy systems, such as decreasing carbon emissions and enhancing energy storage. One example of their successful use is in the efficient and reliable utilization of lithium batteries. In addition to serving as the primary storage method for a decarbonized power system, batteries also hold a significant role in the process of decarbonization [113].

This study builds upon previous successes in using surrogate modelling and ML techniques to represent complex energy systems. The goal is to develop a computationally efficient large-scale electricity system planning ESM that can provide holistic insights and support the attainment of decarbonization goals.

3.2.3 Objectives and Contributions

The objectives of this research are as follows:

1. To develop a computationally efficient ESM to investigate complex relationships within the Canadian electricity system.
2. To leverage the expanded functionality of this modelling approach to produce high-impact insights into key drivers of Canada's decarbonization pathways.

To achieve the objectives of this research, we propose a method to explore the Canadian electricity system design space using an ML surrogate of the Canadian Opportunities for Planning and Production of Electricity Resources (COPPER) model [99]. A computationally efficient model emulating COPPER results enables comprehensive exploration of electricity system relationships. It identifies emergent trends across thousands of optimal solutions. Key factors are identified, input-output correlations are clustered, and sensitive design variables are quantified. This approach supports evidence-based dialogue and informed policies for rapid national-scale decarbonization.

Many of the successful applications of ML to renewable energy systems have focused on analysis with a narrower scope, such as a single technology, sector, or geographical region [5]. To the best of our knowledge, there is not yet any tool that utilizes ML methods to investigate the complex interdependency of factors involved in large-scale energy systems and the efficacy of sustainable energy policies. Therefore, the contributions of this work are as follows:

- We propose a pipeline that utilizes ML methods to reduce the computational burden of a capacity expansion model at a national level by 5 orders of magnitude, with a mean R-squared value of 0.93. Utilizing this tool, we investigate the complex interdependency of factors involved in large-scale energy systems and the efficacy of sustainable energy policies.
- Using this model, we identify key variables affecting power systems and provide sensitivity measures leading to a more robust analysis.
- We implement an easy-to-interpret method utilizing unsupervised ML methods and comparative maps, allowing for the effective conveyance of results to stakeholders.

- We compare the outputs' behavior to changes in all inputs. The impact of all inputs on specific outputs is evaluated with a quantitative metric.
- The results of this study contribute a huge amount of insights into Canada's electricity system development, some of which are further explored and understood through advanced visualizations.

This paper has been divided into 6 sections. Section 2 elaborates on our methodology in utilizing ML methods for exploring the vast design space. In section 3.1, the performance of the surrogate model is assessed in terms of accuracy, speed, and memory usage relative to the base COPPER model. Then in section 3.2, the results are visualized to qualify and quantify the correlations of policy-relevant inputs to emergent system outputs, allowing for the identification of key factors driving emissions and wind and natural gas (gas) generation capacity. The results of the model development process and the ensuing analysis are then summarized, and the implications of this work are discussed in section 4.

3.3 Materials and Methods

In this work, we employed NNs as a surrogate modelling technique to describe the Canadian electricity system.

3.3.1 Electricity system capacity expansion modelling using COPPER

COPPER is a recently developed long-term planning model that determines the least-cost generation and transmission capacity mix over a specified period and timestep. This calculation is based on a predefined set of inputs including projected demand, geographical wind, and solar resource distributions, and modelled policies. COPPER was designed to address research questions regarding various Canadian capacity expansion scenarios. Its objective function minimizes total costs under technical power system constraints, simulating across time steps to chart effective pathways. Scenarios can then be compared through visualizations. It was chosen as the base model for this analysis due to its inclusion of major carbon management policies aimed at reaching Canada's goal of net-zero emissions. The version of COPPER used in this work includes a carbon tax, coal power phase-out, and gas-fired power plant performance standards.

COPPER is a powerful tool for evaluating carbon pricing impacts on future generation mixes [99]. However, its framework is computationally intensive. It is impractical for isolating, quantifying, or ranking the impact of a carbon tax or other policy parameters against other design variables. Running a single scenario can require 16 to 32 CPUs, 64 to 132 GB of memory, and 11-72 hours of computing time. This work uses surrogate modeling techniques to make COPPER more efficient. It explores input sensitivities in the Canadian climate policy design space. This includes the effects of subsidies on technology costs, carbon tax values, and efficiency regulations on demand growth, emissions, and generation capacity.

3.3.2 Surrogate model development with deep neural networks

A NN is a parametric function that transforms an input into a corresponding output. It utilizes stacked layers of linear parametric transforms combined with nonlinear "activation" functions between the layers. Theoretically, NNs can

model any base function with enough parameters [114]. They include complex mappings between inputs and outputs exhibited by energy systems models, with reasonable computation time and high accuracy [115], [116].

NNs with more than two layers are referred to as deep NNs, and each added layer allows the NN to capture more complex mappings. Among the various deep NN architectures introduced in literature [117], residual networks have gained popularity for their performance and ease in training. The core feature of residual networks is the existence of residual (skip) connections between various layers. This enables the NN to learn more intricate relationships [65]. This is particularly crucial when attempting to model complex interdependencies within the electricity system over time, as represented by the COPPER model.

A typical training procedure involves providing the deep network with paired inputs and corresponding outputs. The parameters of the NN are then optimized via gradient-based learning [114] to minimize the discrepancy between the deep network outputs and the supplied outputs. The optimization process typically involves selecting a random subset of the training data, called the training batch, and an optimization process, such as ADAM [114]. This is specifically designed for NN training. We followed standard protocols for deep NN training, as outlined in [115].

3.3.3 COPPER surrogate model development

The model development was carried out in three phases: (1) data generation, (2) data preparation, and (3) model training.

3.3.3.1 Data generation

To train, validate, and test the surrogate NN options, a dataset of COPPER simulations was generated. In this analysis, the carbon tax, capital costs by generation type, and annual demand growth rate by province were selected as the most important design inputs based on optimization constraints in COPPER [99]. These variables represent possible Canadian climate policy pathways; specific carbon tax values, technology subsidies, efficiency regulations, and demand-side interventions. These variables were initially sampled uniformly over predefined ranges listed in Table 1.

Table 1 Simulation dataset input range. The input values for running COPPER are randomly selected in each of these ranges.

Input variable	Range	Unit
Carbon tax	50 - 750	\$/ton
Total demand growth 2050/2018	1.4 – 2.8	Ratio
Annualized capital cost of natural gas	106.687 – 130.396	\$/kW
Annualized capital cost of diesel	159.148 – 194.514	\$/kW
Annualized capital cost of coal	449.183 – 549.00	\$/kW
Annualized capital cost of nuclear	795.514 – 972.295	\$/kW
Annualized capital of cost biomass (waste)	465.161 – 568.531	\$/kW

Annualized capital cost of gas simple cycle (gasSC)	83.478 – 102.029	\$/kW
Annualized capital cost of wind	119.447 – 167.226	\$/kW
Annualized capital cost of solar	85.602 – 142.670	\$/kW

The lower and upper bounds for each input were determined in consultation with subject matter experts. They consider the feasible ranges for policy tuning based on values taken from the paper proposing CREST [23] and COPPER [99]. We increased these values by approximately 25 % for the upper bounds and decreased by approximately 25% for the lower bounds, which is a common practice in sensitivity analysis to cover the whole design space. A carbon tax range was selected based on the minimum and maximum increase in each year present in scenarios developed for COPPER [99]. This encompasses Canada’s “A Healthy Environment and a Healthy Economy” (HEHE) [118] carbon pricing plan. Capital costs are location-specific and exhibit wide variability between studies, so the ranges selected for this analysis were also based on values taken from the papers proposing CREST [23] and COPPER [99]. The ranges for capital costs of wind and solar were chosen to be wider than in [99] in consideration of the uncertainty in the technological evolution of these renewable energy sources and covering the design space. Demand growth varies between provinces and was taken from [23] and [99], and it was also widened by 25% on either side of the nominal value. In COPPER V5 was used in this work, and capital costs and capacity factors are considered constant in each year. This work does not account for technological evolution over time is not accounted for, adding a limitation to the validity of this work.

Next, complete input datasets including the randomly sampled values of the design inputs were used to generate COPPER simulation output datasets. Given the long duration required for COPPER runs, the initial sample size was 1000 datasets, each consisting of a full set of COPPER results in 2030, 2040, and 2050. For dataset generation, we applied the default constraints in COPPER. These conditions include the application of the carbon tax to gas prices; consideration of existing transmission between provinces with no interprovincial transmission capacity expansion; consideration of existing hydro generating capacities with no hydro generation capacity expansion. These constraints were selected to encompass the most practical and non-contentious pathways, as the thorough examination of these matters is not the primary focus of this analysis. Additional information on the parameters used in the COPPER model can be found in reference [99].

The training dataset was derived from the COPPER simulation results. Specifically, the annual carbon emissions by province and the capacity for wind and gas at both the provincial and national levels were isolated. These variables were chosen as they are crucial indicators of interest in policy formulation.

3.3.3.2 Data Preparation

The data were preprocessed for NN training through cleaning, normalization, and standardization. Firstly, the model outputs were cleaned up by removing the missing values (NaNs), constant values, and the output data outliers based on a 5-sigma margin. Next, outputs were standardized based on their mean and standard deviation, to increase the

speed of model training and give equal weight to all the model outputs. Additionally, variance clipping was applied to the model outputs; where values with a standardized variance of less than 0.001 were considered model noise and excluded from the training process. The model inputs were normalized based on their maximum and minimum values such that all inputs are in the range of 0 to 1. The data set of COPPER simulations was generated and split into training (80%), validation (10%), and testing (10%) subsets. Normalization of inputs and standardization of outputs were performed as per eqns. (1) and (2), respectively:

For i in X :

$$\hat{x}_i = \frac{x_i - \min(x_i)}{\max(x_i) - \min(x_i)} \quad (1)$$

For i in Y :

$$\hat{y}_i = \frac{y_i - \text{mean}(y_i)}{\text{std}(y_i)} \quad (2)$$

3.3.3.3 *Model training*

The model training algorithm aimed to minimize the loss function, which was defined as mean-squared error (MSE) between the NN output predictions and the provided data (calculated using eqn. (3)). Lower MSE values are indicative of greater model accuracy. To prevent overfitting, the training and validation losses were compared during the model tuning process. The NN architecture was selected based on empirical experimentation, by ensuring that the validation loss did not increase over additional training epochs. The model training platform was developed with the PyTorch Lightning library in Python [119], and it was executed on a Graphics Processing Unit provided by Compute Canada.

$$MSE = \frac{1}{n} \sum_{i=1}^n \left(Y_i - \hat{Y}_i \right)^2 \quad (3)$$

3.3.3.4 *Ablation study to determine model architecture*

We experimented with a multi-layered NN architecture featuring residual blocks [65] to regress the model outputs against the training dataset. The key design choices in model architecture are the number of layers and neurons per layer, activation function (sigmoid, ReLu, hyperbolic tangent, etc.), batch size, and learning rate [114]. Dropout was used to reduce the risk of overfitting by random omissions of neurons during a neural network's training process [120]. A detailed examination of the impact of changes in design parameters on the model's performance is provided

in Table 2, which presents a selection of high-accuracy architectures identified during the experimental process, along with their corresponding prediction errors.

Table 2 Model architecture experiment – a sample of higher accuracy architectures and associated prediction errors for training and test datasets

Architecture	Training error (MSE loss)	Test error (MSE loss)
1 linear + 12 Residual blocks, Neurons per block = 128, Dropout ratio = 0.5 Batch size = 128, Learning rate = 0.001	0.010	0.049
1 linear + 13 Residual blocks, Neurons per block = 128, Dropout ratio = 0.5 Batch size = 128, Learning rate = 0.001	0.018	0.06
9 linear blocks, Neurons per block = 128, Dropout ratio = 0.5 Batch size = 128, Learning rate = 0.001	0.012	0.08
10 linear blocks, Neurons per block = 128, Dropout ratio = 0.5 Batch size = 128, Learning rate = 0.001	0.02	0.09
1 linear + 12 Residual blocks, Neurons per block = 128, Dropout ratio = 0 Batch size = 128, Learning rate = 0.001	0.05	0.1
1 linear + 12 Residual blocks, Neurons per block = 128, Dropout ratio = 0.5 Batch size = 128, Learning rate = 0.001	0.04	0.09
1 linear + 12 Residual blocks, Neurons per block = 512, Dropout ratio = 0.5 Batch size = 128, Learning rate = 0.0001	0.03	0.1
1 linear + 12 Residual blocks, Neurons per block = 512, Dropout ratio = 0.5 Batch size = 128, Learning rate = 0.01	0.06	0.09

Finally, the model architecture with 12 residual blocks was selected. Each block consists of two linear layers, two batch normalizations, two ReLu activation functions, and two dropout layers. This model is summarized in Table 3, and its architecture schematic is shown in Figure 8.

Table 3 Selected model architecture with the highest accuracy

Architecture

1 linear + 12 Residual blocks

Neurons per block = 128

Dropout ratio = 0.5

Batch size = 128

Learning rate = 0.001

25k steps (2000 epochs)

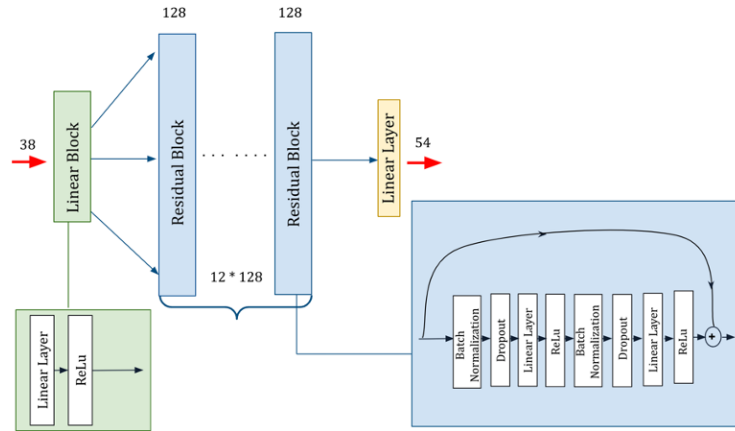


Figure 8 Schematic of the architecture of the model – dimension and structure of layers – the model has a linear block containing a linear layer and ReLu activation function followed by 12 residual blocks - each block containing two batch normalizations, two dropout layers, two ReLu activation function, and two linear layers and the last layer is a linear layer – dimension of input and output layers are 38 and 54 respectively which is the number of selected inputs and outputs of COPPER.

3.3.4 Exploring correlations in the design space

The proposed model was used to analyze the design space, quantify correlations between outputs and inputs, and identify key factors affecting model results. Correlations between each input and output were investigated using the COPPER surrogate model. The inputs were randomly sampled 1000 times from a uniform distribution, with one input being varied randomly while the other inputs were kept constant at their respective mean values. The outputs of the surrogate model were then calculated, recorded, and plotted against the chosen input variable. This process generated more than 2000 plots, which collectively illustrate interdependencies between inputs and outputs. Due to the scale of this analysis, a pipeline was implemented to process results effectively and identify key insights. Two analytical and visualization techniques were applied to communicate the findings:

1. Clustering and mapping input-output relationships onto heat maps to provide qualitative depictions of the strength of each correlation.
2. Charting the normalized maximum derivatives of two key outputs in each time step with respect to each input as a supplementary indicator showing the relative quantified impact of all inputs on a target output.

3.3.4.1 Clustering and dimensionality reduction of the results

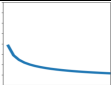
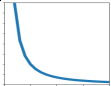
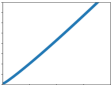
We used clustering and dimensionality reduction techniques to group similar relationships that were found between each input and output. This allowed us to identify strong or surprising correlations among the 2000 plots more efficiently, rather than having to review each one individually.

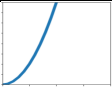
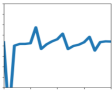
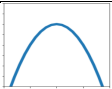
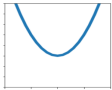
Clustering is a data analysis technique used to group similar subgroups (clusters) in the dataset. Firstly, we used the k-means algorithm to group data points based on their similarity in terms of shape. This allows us to quantify correlation and identify the key factors that affect the model results. K-means is an unsupervised ML algorithm that iteratively identifies k distinct, non-overlapping clusters within the data set such that each datum can be assigned to a group. The pattern of change (increase, decrease, etc.) in input-output variation can then be identified through observation for each grouping.

After clustering the data, we used visualization techniques to help identify the unique relationship of each group. We used the t-distributed stochastic neighbor embedding (t-SNE) technique [56]. It is a dimensionality reduction method that maps the high-dimensional data to a 2D plot, making it easier to visualize and understand the multidimensional clusters. This technique helped us to more easily identify the characteristic relationship of each group.

Then, the characteristic relationships observed within each group were labeled to facilitate the interpretability of the large quantity of information to stakeholders effectively. Eight distinct input-output relationship types were identified, as summarized in Table 4.

Table 4 Input-output relationship types and interpretations

Shape	Sample plot	Interpretation
Negative		The output will decrease with the selected input.
Strongly negative		The output will rapidly decrease with the selected input.
Relatively insensitive		The output's variation with respect to the input is not significant relative to its variation with respect to other inputs. Note that these values are normalized, so this does not necessarily imply there is a constant relationship.
Positive		The output will increase with the selected input.

Strongly positive		The output will rapidly increase with the selected input.
Inconclusive (unknown)		There is no identifiable pattern in the correlation between the input and the output.
Bell-shaped		The output increases, peaks, and then decreases with respect to the input.
Inverse bell-shaped		The output decreases, reaches a trough, and then increases with respect to the input.

3.3.4.2 *Relative impact of policy parameters*

To quantify the relative impact of specific input parameters on selected outputs, we employed a mathematical technique. It is known as maximum absolute derivatives of standardized outputs with respect to each normalized input. This method provides a quantitative measure of the relative influence of each input parameter on the selected outputs by determining the peak sensitivity of an output to variations in specific input parameters. Calculation of maximum derivatives is a computationally demanding process that is made feasible using a surrogate model. We chose two outputs, wind and gas capacity over time, for this analysis as they are indicative of successful decarbonization in future energy system capacity expansion. The normalized maximum derivatives for these outputs with respect to all inputs were visualized using bar charts. The bar charts are used to identify which inputs have the greatest impact on these outputs, thus providing insights on how to achieve decarbonization.

3.4 Results

The results of this work are presented in two sections. The first section covers the results of the surrogate model development, including the model evaluation, performance, and limitations. The second section presents the results of the analysis that was conducted using the proposed model.

3.4.1 COPPER surrogate model performance

In this section, we evaluate the results, performance, and computational cost of the surrogate model in comparison to the actual COPPER model and point out the limitations of the surrogate model. This section of the results will help to determine how well the surrogate model approximates the actual COPPER model. They also help to identify any output where the surrogate model may not be as accurate or efficient as the actual model. This comparison will give an idea about the validity of the proposed model and its limitations.

3.4.1.1 *Model evaluation*

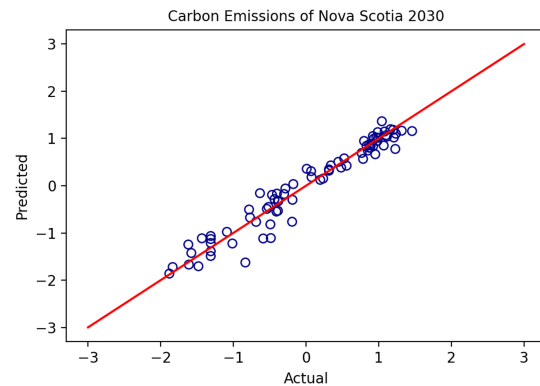
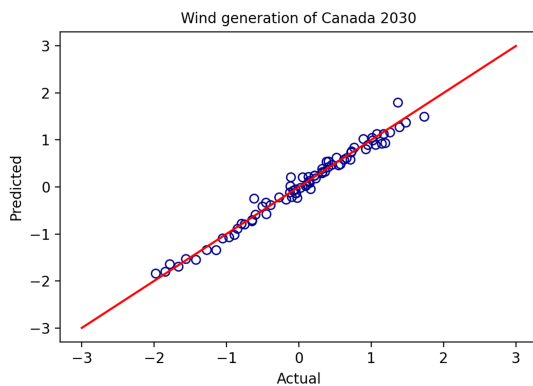
A lower MSE loss generally indicates greater accuracy in predictions during model tuning. However, it is not clear what MSE loss value should be considered a sufficiently close approximation of the base COPPER model. To resolve this, we assess the quality of the output regressions. It means comparing the results of the surrogate model with the actual results of COPPER, to evaluate the quality of the prediction. For each ML model output, we generated a scatter

plot for comparison to the same output from the test dataset. An ideal surrogate model would produce diagonal lines with R-squared values of 1 for all plots. As a secondary metric, we report the minimum R-squared value overall output regression plots and set an acceptance threshold of 93%.

Table 5 reports the performance results of the proposed model, including training, validation, and test errors, as well as the R-squared value for the test data set. The R-squared value is a measure of the goodness of fit of the model, with a value of 1 indicating a perfect fit and a value of 0 indicating no fit. For each datum in the test dataset, R-squared is calculated, and then the minimum, maximum, and mean are calculated over the test dataset. This table shows the R-squared distribution statistics with a mean of 0.93 for all regressions. These results give an overall idea of how well the model is performing on various data sets. Figure 9 shows six selected regression plots out of 54 with the minimum, maximum, and mean R-squared for the unseen test data set. These figures demonstrate that even in cases where the R-squared value is low, the model still achieves a high degree of accuracy in its predictions. Note, all values are normalized in the figure to facilitate visualization.

Table 5 Performance of the proposed model in terms of MSE losses and R-squared distribution for the test data set

Training loss	Validation loss	Test loss	Mean R-squared	R-squared standard deviation
0.01	0.047	0.049	0.93	0.05



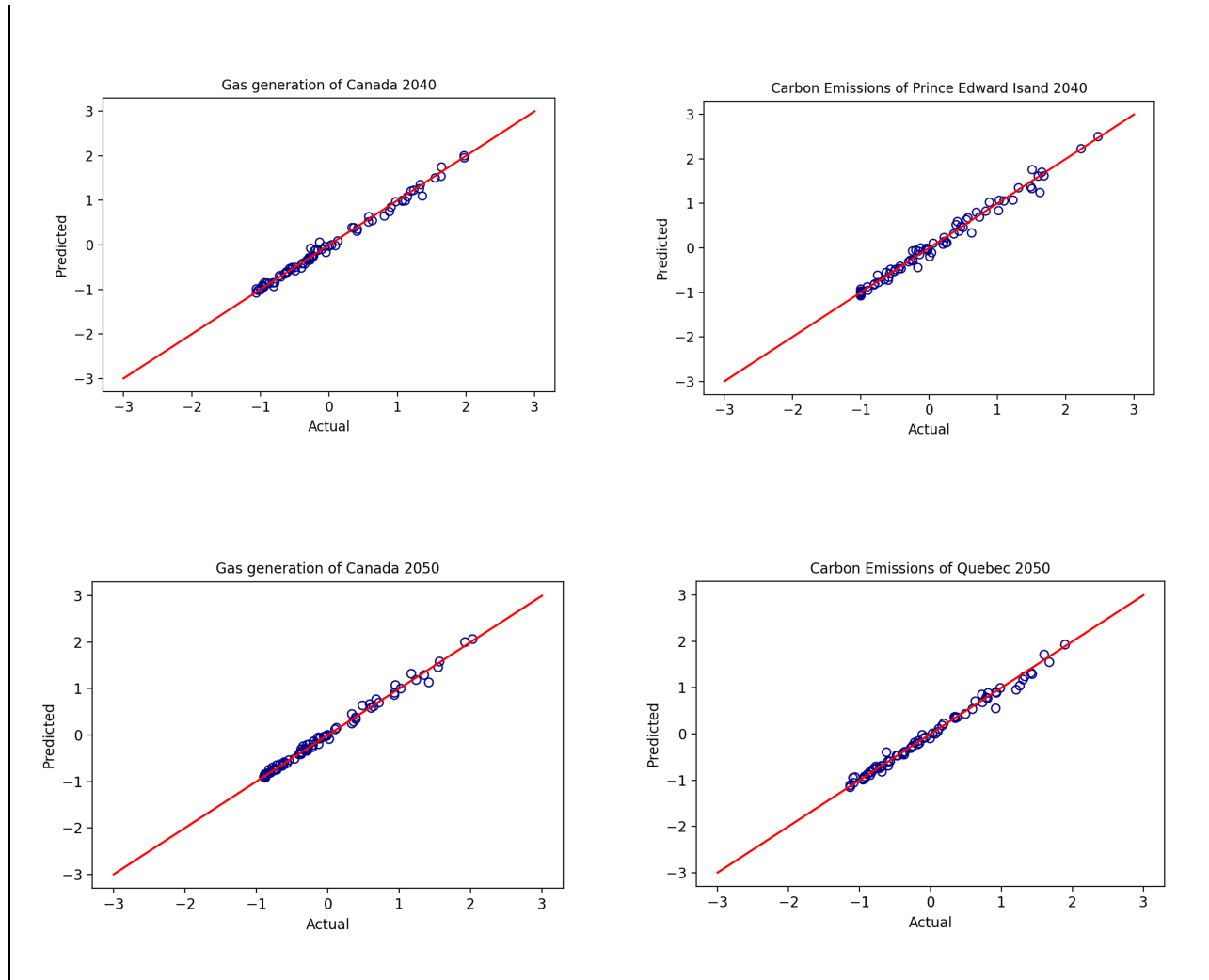


Figure 9 The selected regression plots – they show the relationship between the outputs of the proposed model and the actual values of the test data set. The X-axis represents the actual values of COPPER results, while the Y-axis represents the predicted values of the surrogate model. The red line ($x=y$) corresponds to the highest level of accuracy, where the predicted and actual values are the same. The closer the blue dots are to the red line, the more accurate the predictions of the model are. These plots allow for visualization of the model's performance and can be used to identify outputs where the model may not be performing as well.

3.4.1.2 Computational cost evaluation

Table 6 compares the run-time and required resources of the proposed model against COPPER to evaluate the computational cost of the model. The results show a significant reduction in computational time and required resources when using the proposed model. These results are important for a wide range of applications, as the reduction in computational time and resources can lead to cost savings and make the model more accessible to a broader range of users.

Table 6 Comparison of COPPER and proposed model computational costs and run time

Model	CPU	Memory	Run-time
COPPER	16 – 32	64 – 128 GB	11h – 72h

Residual neural network	1	NA *	17.1 millisecond
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* Except for saving the model and associated data.

3.4.1.3 *Limitations of machine learning models for surrogate energy systems analysis*

The developed model is less sensitive to parameters with relatively small nominal values across its variation range. This is because these small values approach zero when the input dataset is normalized, leading to their contribution to the MSE in the network being relatively small. As a result, the relative inaccuracy of small values is not a large driver of network optimization or architecture choices, and it is not captured in an overall accuracy metric. This means that the corresponding prediction accuracy for small-valued outputs may be lower than for larger-valued outputs. This is particularly relevant for parameters where there are small variations between provinces. This limitation should be considered when interpreting the results of the model and when making predictions for small-valued parameters. For example, the annual carbon emissions in Nova Scotia are much lower than in Alberta due to differences in population and the carbon intensity of their power grids. Because the model is less sensitive to small values and variations, the predictions for Alberta will tend to be more accurate than for Nova Scotia. This is a common limitation of ML. To overcome this limitation, one could consider collecting more data specific to Nova Scotia or use different techniques such as weighting the loss function to give more importance to specific regions like Nova Scotia or Alberta.

Another limitation of the surrogate model relates to the wider range of inputs that can be changed in COPPER for the purpose of exploring specific scenarios of interest or adding new constraints. In contrast, this surrogate model is limited to the initial input selection chosen for this work. To address this limitation and the uncertainty associated with future capital costs in future work, the selected variation ranges can be widened such as $\pm 50\%$ instead of $\pm 25\%$. Or the analysis could be preceded by a systematic literature review of capital cost projections that were considered beyond the scope of this analysis.

Furthermore, as COPPER improves and more features are added, the NN will need to be retrained to continue to accurately model the Canadian electricity system. It includes the computational cost of producing and updating the training data and retraining the model. For example, we used COPPER V5 for our model development, in which uncertainty of capital costs is not considered and they are constant for each year. But in the latest version of COPPER technology evolutions are considered and capital costs are not constant. Therefore, this model will need to be retrained and updated as COPPER evolves to ensure its continued accuracy.

There are caveats associated with the analysis conducted in this work relative to standard sensitivity analysis methods:

There is an inherent level of error (correlations aren't $R_{\text{squared}} = 1$), so it is unclear to what extent the model can accurately reproduce sensitivities.

The input parameters are varied one-at-time (OAT), and this is not considered suitable for sensitivity analysis for a non-linear system. For a non-linear system, a more appropriate sensitivity analysis method would be global sensitivity analysis, which considers the interactions between inputs and can provide more accurate results.

3.4.1.4 Limitations relative to COPPER for policymakers

Finally, the surrogate modelling methodology used in this work has some limitations relative to the base COPPER model in relevance, intelligibility, and validity.

Firstly, the systematic errors identified above demonstrate that the surrogate model is useful for identifying strong key relationships rather than specific numeric results. So, the base COPPER model is more suitable to use in policy design projects where there are numeric objectives. Similarly, the surrogate is the most successful at capturing large values. This led to it producing the most accurate predictions for larger provinces and limiting its relevance in smaller jurisdictions.

Secondly, due to the comparative nature of this analysis and the use of normalized data to generate model outputs results in analysis where all findings are relative, and no numeric results descriptive of the real system are presented in this work. As such, the surrogate lacks some of the intelligibility of the base model, and the values must be unnormalized to be interpreted in the context of the real system.

Finally, the linear programming method used by COPPER has structural validity that the surrogate does not inherently have, as the deep NN structure of the model does not reflect the structure of the real system. Further validation steps must be taken before results developed using this model are implemented.

Each of these limitations could be addressed by simulating with COPPER to replicate key results found using the surrogate model and validating that the simulation results agree with the surrogate results. Then, these simulation results could be used for detailed and nominal value-based policy planning activities more akin to typical COPPER uses.

3.4.2 Key relationships in Canada's electricity system design space

The use of the surrogate model enabled the evaluation of the changes in system outcomes for variations in policy design inputs in the electricity sector design space. A broad array of insights can be drawn from this analysis about Canada's mid-term electricity sector decarbonization options. They include findings regarding the effects of demand growth, technology costs, and carbon taxes in each province between the present time and end dates corresponding to the Paris Agreement targets.

The analysis firstly presents the relationships in a heat map format where the color corresponds to the nature of the relationship. This makes it easy to identify the strongest relationships affecting key system indicators at each timestep. This also allows for a clear visual representation of the data and facilitates the identification of key relationships. Secondly, the outputs' maximum derivatives with respect to each input are provided as a quantitative metric for understanding the relative importance of policy-relevant inputs for the capacity expansion of gas and

wind generation. This allows for a more in-depth understanding of the impact of different inputs on the electricity sector, providing valuable insights for decision-making and policy-making.

3.4.2.1 Correlations between inputs, and emissions and generation output

The heat maps depicting the characteristic relationship between each input and each output for the years 2030, 2040, and 2050 are presented in Figure 10, Figure 11, and Figure 12, respectively. They provide a visual representation of how each input affects each output at different timesteps.

The heat map grid size (i.e., the number of input and outputs for which a relationship was classified) vary over the considered timesteps. Because, as stated above, values that are constant or have very small variations in the training dataset at a timestep were removed from model training process during data preparation based on 5-sigma threshold for standard deviation. In other words, if any selected design output was not associated with relatively significant variation in COPPER simulations, it has been excluded from the surrogate model calculations.

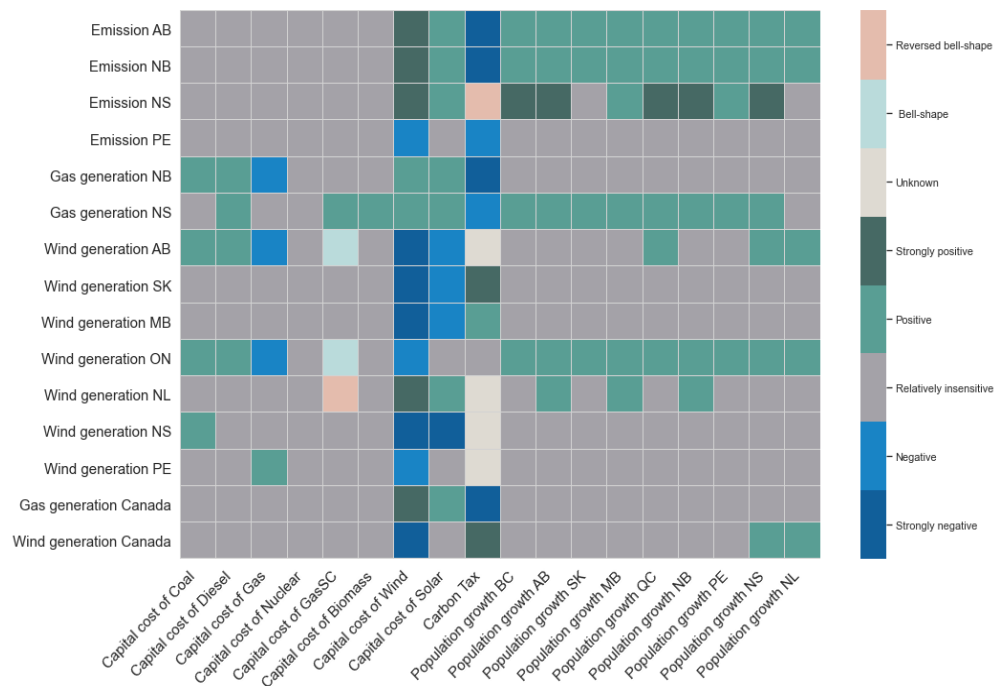


Figure 10 This heat map shows the relationship between the inputs (X-axis) and outputs (Y-axis) in 2030. It includes only design variables that have variations in the training dataset. The correlations are color-coded based on the shape of input-output correlation plots. The plots are scaled for each output based on the minimum and maximum values, so the relationships

depicted in the heat map are relative to the specific output being considered. The heat map provides a visual representation of how each input affects each output and allows for easy identification of the strongest relationships.

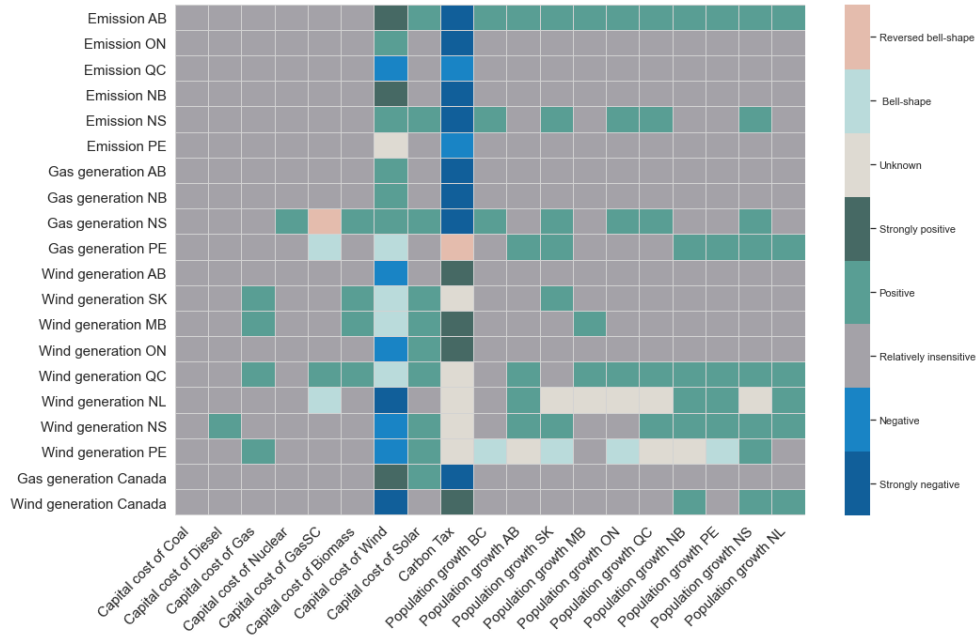


Figure 11 This heat map shows the relationship between the inputs (X-axis) and outputs (Y-axis) in 2040. It includes only design variables that have variations in the training dataset. The correlations are color-coded based on the shape of input-output correlation plots. The plots are scaled for each output based on the minimum and maximum values, so the relationships depicted in the heat map are relative to the specific output being considered. The heat map provides a visual representation of how each input affects each output and allows for easy identification of the strongest relationships.

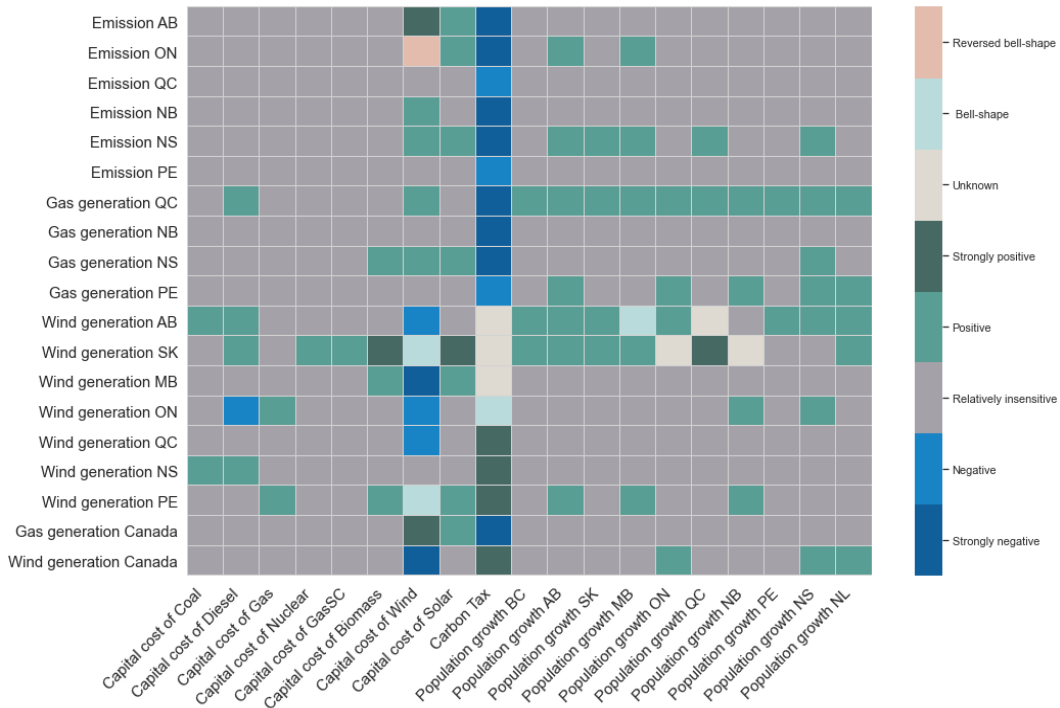


Figure 12 This heat map shows the relationship between the inputs (X-axis) and outputs (Y-axis) in 2050. It includes only design variables that have variations in the training dataset. The correlations are color-coded based on the shape of input-output

correlation plots. The plots are scaled for each output based on the minimum and maximum values, so the relationships depicted in the heat map are relative to the specific output being considered. The heat map provides a visual representation of how each input affects each output and allows for easy identification of the strongest relationships.

The heat maps present a large amount of information that can be interpreted by analyzing and comparing the pattern of change in output values given variation for each input variable. This clustering can provide valuable insights into the types of relationships between policy inputs and system outcomes. However, the surrogate analysis generates a large amount of information, and it would not be feasible to explore every relationship in depth in this work. Therefore, this analysis should be considered as a starting point for further research to identify the most important relationships and their implications.

The results suggest that the carbon tax is the most influential determinant of Canadian electricity system outcomes between now and 2050. The carbon tax level is strongly negatively associated with emissions in most provinces at all time steps. This confirms the importance of Canada's federal-level commitment to carbon pricing policies, such as the Pan-Canadian Approach to Carbon Pollution Pricing [121].

The results further suggest that wind is the renewable energy source with the greatest influence on Canada's electricity grid development, particularly for 2030. The capital cost of wind is shown to be positively correlated with emissions in some provinces and negatively correlated with built wind capacity in most provinces. Of all the renewable energy subsidy options, this analysis suggests that reducing the capital cost of wind across Canada results in the greatest emissions reductions. This is a crucial insight for Canada's 2030 electricity system greenhouse gas targets, as it highlights the importance of reducing the cost of wind energy to achieve emissions reduction goals.

3.4.2.2 *Ranking of factors affecting gas and wind capacity development*

In this section, we explore the factors that determine the expansion of gas and wind energy generation capacity at the national scale. These key outcomes do not directly correspond to current Canadian policy targets, such as annual GHG emissions. However, they are responsible for significant contributions to Canadian energy generation and are indicative of either the continuation of business-as-usual or realized decarbonization efforts. By understanding the determinants of these outcomes, policy makers can identify the most effective policies and strategies to promote decarbonization in the Canadian electricity sector.

The analysis of system parameters and their potential impact on the future supply mix in Canada is represented by the maximum derivatives of gas and wind capacities with respect to each input. These values are normalized to determine the relative impact of each variable and are used to rank policy options based on their relative impact. The negative values show the negative correlations, positive values show positive correlations, and the absolute values of maximum derivatives represent the correlation intensity. The results are displayed in bar charts for Canada for the years 2030, 2040, and 2050 in Figures 13-15, respectively. They provide a clear visual representation of the relative importance of each input variable in determining the expansion of gas and wind energy generation capacity. This information can help policy makers identify the most sensitive parameters and prioritize efforts to achieve decarbonization goals.

National Gas and Wind Generation Capacity in 2030

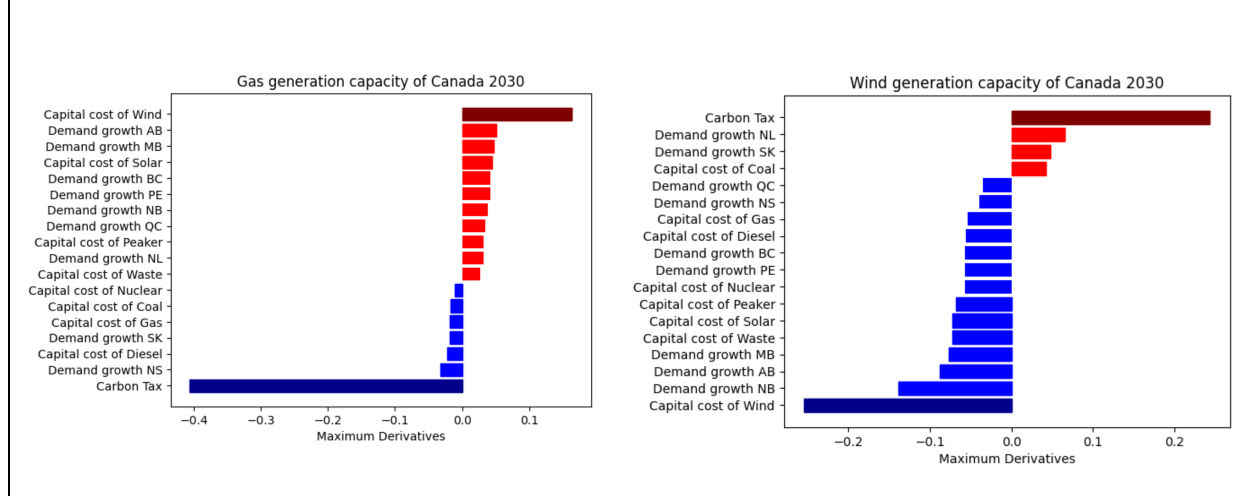


Figure 13 Ranked factors affecting Canadian gas and wind generating capacities in 2030 are presented in bar charts. These are quantitative measures of the relative impact of system inputs on two key components of the Canadian energy supply mix, with the parameters listed on the Y-axis. These values, which show correlation intensity, are normalized maximum derivatives of gas and wind capacities with respect to each input on the Y-axis. The negative values show the negative correlations, positive values show positive correlations, and the absolute values of maximum derivatives represent the correlation intensity.

National Gas and Wind Generation Capacity in 2040

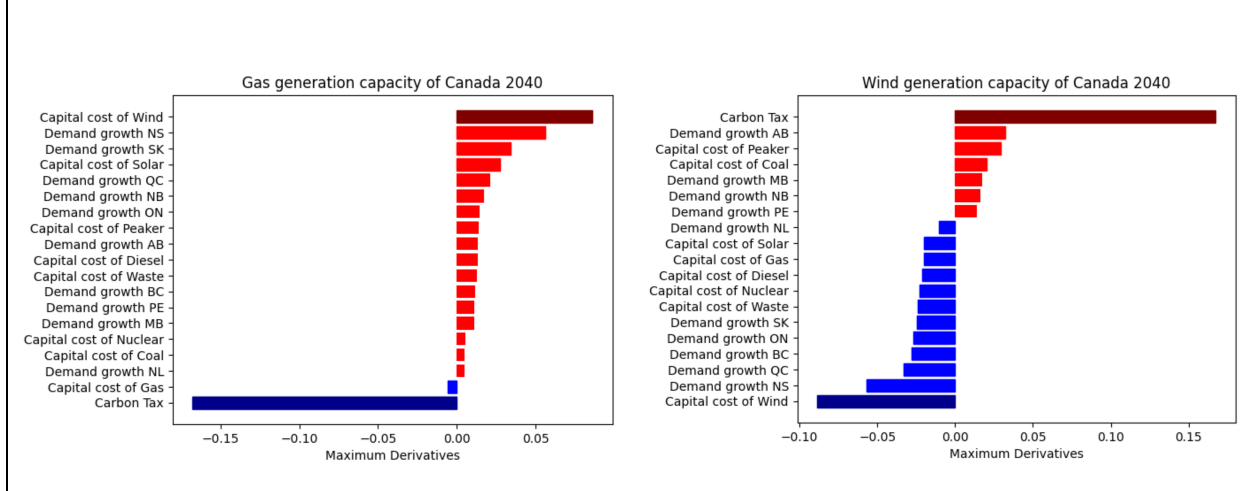


Figure 14 Ranked factors affecting Canadian gas and wind generating capacities in 2040 are presented in bar charts. These are quantitative measures of the relative impact of system inputs on two key components of the Canadian energy supply mix, with the parameters listed on the Y-axis. These values, which show correlation intensity, are normalized maximum derivatives of gas

and wind capacities with respect to each input on the Y-axis. The negative values show the negative correlations, positive values show positive correlations, and the absolute values of maximum derivatives represent the correlation intensity.

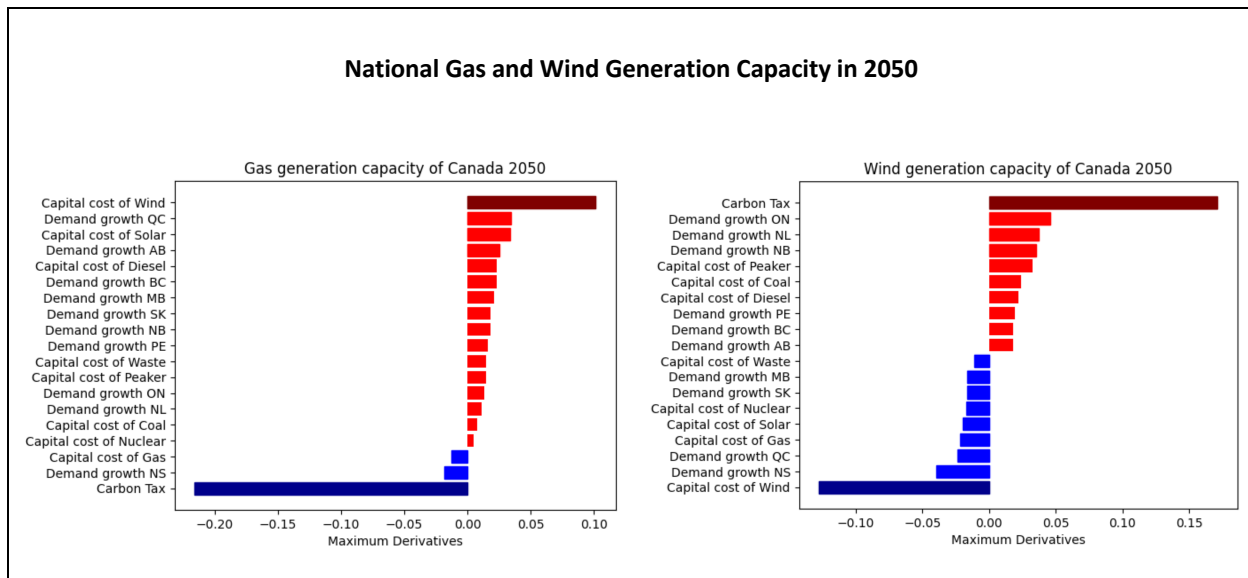


Figure 15 Ranked factors affecting Canadian gas and wind generating capacities in 2050 are presented in bar charts. These are quantitative measures of the relative impact of system inputs on two key components of the Canadian energy supply mix, with the parameters listed on the Y-axis. These values, which show correlation intensity, are normalized maximum derivatives of gas and wind capacities with respect to each input on the Y-axis. The negative values show the negative correlations, positive values show positive correlations, and the absolute values of maximum derivatives represent the correlation intensity.

The results reinforce the previously mentioned findings that the most influential determinants of Canadian electricity system outcomes between now and 2050 are the carbon tax and the capital cost of wind. The capital cost of wind plays a particularly significant role, exhibiting a relative impact on the expansion of gas and wind capacities four times as large as any other technology cost. The results show that across all time steps, changes in other demand growth and non-wind energy technology cost parameters have minimal effects on the development of wind and gas generation capacities.

3.5 Discussion

We find that there is a broad array of holistic insights we can draw from this surrogate model by clustering or by ranking each correlation, and then comparing these relationships across years, provinces, or parameters. The results confirm the effectiveness of policies such as carbon pricing and wind subsidies and highlight their significance compared to other options. The remainder of the analysis will focus on the most notable findings from national-level results.

3.5.1 Demand growth effects

The analysis shows that the relationship between electricity demand and emissions is not consistent across provinces and over time. An increase in demand growth rate will lead to an increase in carbon emissions in most provinces, in New Brunswick and Nova Scotia until 2030 and Alberta until 2040. Of particular interest are the highly positive and

positive correlations, respectively, between emissions and gas generation capacity, and demand growth in many of the provinces with the highest populations (i.e., BC, AB, QB) and Nova Scotia. This uneven distribution suggests tailoring policies to each province's needs. Efficiency measures, renewable energy expansion, and stricter renewable portfolio standards should align with provincial specifics when implemented locally.

3.5.2 Capital cost effects

The capital cost of non-renewable energy technologies, including nuclear energy, does not have a significant impact on emissions. Because carbon pricing is already high enough that non-renewable sources cannot compete with renewable sources in terms of cost. However, the capital costs of solar and wind energy have a significant impact on Canada's electricity system development. They are negatively correlated with emissions and gas capacity in many provinces. This suggests that policies aimed at reducing the cost of renewable energy technologies can effectively reduce reliance on additional gas generation capacity, particularly in New Brunswick and Nova Scotia. Climate policy that raises the capital cost of coal and diesel raises wind capacity in some provinces but also increases gas capacity in other provinces, highlighting the importance of considering localized impacts when implementing federal-level policies like a coal phase-out.

3.5.3 System sensitivity over time

The sensitivity analysis of COPPER, a model used to simulate the electricity sector under a net-zero constraint, shows that the system's outputs become more stable over time as the grid approaches the net-zero constraint. The greatest variation in emissions and generation mix is seen in 2030, with the impact of changes in demand growth being the highest. By 2040, technology capital costs become less of a determinant of emissions and generation capacities. The system is less susceptible to diverse outcomes due to changes in parameters. This finding aligns with prior COPPER simulations. They show carbon-intensive generation (coal, diesel) should be phased out by 2030. This prevents continued usage into 2050, given their 20–25 year life cycle [99]. This confirms that the most important period for government intervention, decarbonization policies, and green investment is within the next decade.

3.6 Conclusion

The COPPER model handles high-resolution spatiotemporal constraints and detailed policy options. However, its computational burden limits its usability. The ESM developed in this work addresses this by efficiently exploring the electricity sector's design space. It characterizes relationships between policy inputs and system outcomes across thousands of model runs. Efficient computational techniques used here have not been applied to large-scale ESMs before.

The proposed deep NN pipeline reduced computational time and resource requirements by 5 and 6 orders of magnitude, respectively. It only requires a single CPU while maintaining high accuracy (mean test regression R-squared of 0.93). This resolves the computational limitations of the COPPER model.

The surrogate model produced over 2000 input-output correlation plots. To communicate these insights, a visualization method using K-means clustering, heat maps, and ranked bar charts was developed. This tool enables

stakeholders to easily derive holistic insights, guiding policymakers with quantitative metrics for effective electricity system decarbonization planning. The analysis highlighted key system relationships and determinants of critical components in the electricity supply mix.

The rapid evaluation enabled by this low-burden model allowed exploring new research questions and Canada's electricity system design space. The analysis found that carbon taxes and wind capital costs are the most impactful parameters for electricity system outcomes, including emissions reductions in many provinces. This finding supports Canada's carbon pricing plan as the most effective policy for decarbonizing the electricity sector.

Reducing wind capital costs was identified as an effective secondary strategy for emissions reduction. Research and policy support in this area should be prioritized in the near term. Maximum derivatives analysis showed that increasing carbon pricing and reducing wind costs are the most effective measures for increasing wind capacity and reducing gas capacity. Carbon taxes had up to four times the impact of wind cost reductions, while wind costs had twice the impact of any other energy technology cost. These interventions are significantly more impactful than policies affecting other technologies or demand growth.

The analysis highlighted localized effects of demand growth rate changes and the limited impact of increasing non-renewable energy costs. It emphasized the importance of the next decade for electricity system development and decarbonization. These findings underline the need to account for regional variations and act urgently to achieve effective decarbonization.

This work focuses on Canada's future electricity system modeled by the COPPER ESM, offering insights for policy decisions supporting GHG reduction goals. The surrogate modeling methodology developed here is generalizable. It can be applied to other large-scale ESMs to address design, optimization, and robustness questions across various scopes, as demonstrated in other fields using surrogate modeling techniques [6]. Our method was used to develop a set of insights for policy decisions toward Canada's GHG emission reduction goals.

3.6.1 Future work

The findings from this ESM surrogate have implications for future research. This includes reversing the normalization process to explore relationships in real-world contexts. The low-burden ESM can be used to identify optimal input variables for policy planning. A more comprehensive uncertainty analysis and global sensitivity analysis should also be conducted. Expanding the selected ranges by $\pm 50\%$ can analyze uncertainties related to technology evolution over time.

Future development of large-scale surrogate ESMs could address limitations identified in this work. These include using feature scaling to account for magnitude differences in training data. Retraining the model to incorporate new features added to COPPER is another area for improvement.

3.7 Author Contributions

Zahra Jahangiri: contributed to conceptualization, methodology, software, validation, formal analysis, investigation, writing (original draft preparation), writing (review and editing), and visualization. **Mackenzie Judson:** contributed to conceptualization, writing (original draft preparation), and writing (review and editing). **Kwang Moo Yi:** contributed to supervision, resources, writing (review and editing). **Madeleine McPherson:** contributed to supervision, resources, writing (review and editing), and funding acquisition.

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4 Chapter 4: Machine Learning-based Uncertainty Analysis in Power system Planning: Insights and Pathways for Decarbonization

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Zahra Jahangiri, Mohammad Miri, Kwang Moo Yi, Madeleine McPherson
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4.1 Abstract

This study performs an uncertainty analysis of decarbonization pathways for the Canadian power system. Using machine learning (ML) techniques, it represents complexities and nonlinear behaviors of the power system, which are challenging to observe using traditional modeling methods due to computational limitations. We further utilize K-means clustering and statistical methods to identify correlations, investigate the effects of uncertainty in key parameters (capital costs, demand, and carbon tax), and identify opportunities for diversification of the power generation mix. Key findings include the increased flexibility of gas combined cycle (generation mean 4.8 TWh, installed capacity mean 4.8 GW) over gas simple cycle (generation mean 22.3 GWh, 0 installed capacity) in response to carbon tax, highlighting its role in a low-carbon future. Variations in solar and wind deployment rates, influenced by capacity factors and location-specific costs, underscore the necessity of a flexible grid system. This analysis reveals important correlations between renewable deployment, and transmission expansion and gas combined cycle reliance. The results also highlight minimal sensitivity of hydroelectric power generation (~ 43 % of scenarios) to changes in input parameters. The novelty of our work lies in proposing a comprehensive approach which uses ML techniques to go beyond the capabilities of existing models. Specifically, by performing extensive uncertainty analysis and provides key insights into system behavior, causative factors, and an expanded breadth of potential pathways. Taken together, this proposed approach lays a foundation for strategic planning and policy formulation.

Key words: Uncertainty analysis, Machine learning, Energy system planning, Renewable energy

4.2 Introduction and Background

The decarbonization of power grids represents a monumental challenge in the field of energy systems due to its complexity. These systems integrate renewable energy, metering infrastructure, energy storage, and real-time data analytics. These components must operate together to ensure reliability, efficiency, and resilience. Transitioning to renewable resources adds variability and uncertainty, increasing the system's complexity [3].

Understanding these complexities, as outlined by Giampietro et al. [4], is critical for effective policymaking, increasing both resilience and reliability. Identifying leverage points, or human-controllable parameters that can influencing system behavior [51], is essential for guiding energy system transformations.

4.2.1 Modeling Process Diagram

Quantitative models serve as simplified representations of real-world systems, focusing on selected aspects while disregarding others. They have inherent prediction error and are valid only within specific boundaries. These

boundaries are defined by key variables, relationships, and boundary conditions, creating a "finite descriptive domain" [122], [123], [124]. The arbitrary process of creating a model is influenced by modeler bias and methodological limitations. This leads to varying degrees of abstraction from the actual system. This can be increased further by methods used to improve computational tractability. For instance, surrogate modeling, which focuses on isolating crucial parameters and replicating relationships. This approach introduces additional error but improves computational efficiency. Balancing efficiency and precision requires careful evaluation and selection based on analytical goals. Although models have inherent shortcomings and cannot perfectly reproduce real-world behavior, they nevertheless can be used to provide valuable insights into complex systems. As statistician George Box [125] famously said, "all models are wrong, but some are useful."

These considerations are particularly relevant when researching complex socio-technical systems, whose stochastic nature emphasizes the need for uncertainty analysis. Models are subject to both aleatory and epistemic sources of uncertainty. As such, analyzing model results requires explicit and adequate treatment of these uncertainties. Increasingly, uncertainty and sensitivity analysis emerging as key components of uncertainty management in modeling best practice. Monte Carlo simulation, ensemble modeling, and related methods, commonly used in fields such as meteorology, offer comprehensive approaches to uncertainty analysis. Notably, the study of future energy transitions is in its early stages [4], [126], uncertainty analysis is set to play a vital role in providing realistic assessments of future scenarios, acting as a bridge between complex system modeling and effective planning.

Uncertainty analysis evaluates the variability of model outputs to characterize potential behaviors of the system. It quantifies uncertainties in outputs caused by input parameters and modeling assumptions. This process identifies plausible ranges and probability distributions of outcomes. Additionally, uncertainty analysis is a prerequisite to sensitivity analysis, which maps causal influences between input and output uncertainties [127], [128]. Figure 16 provides a visual representation of the relations between real-world systems, models, and approaches to uncertainty discussed in this section.

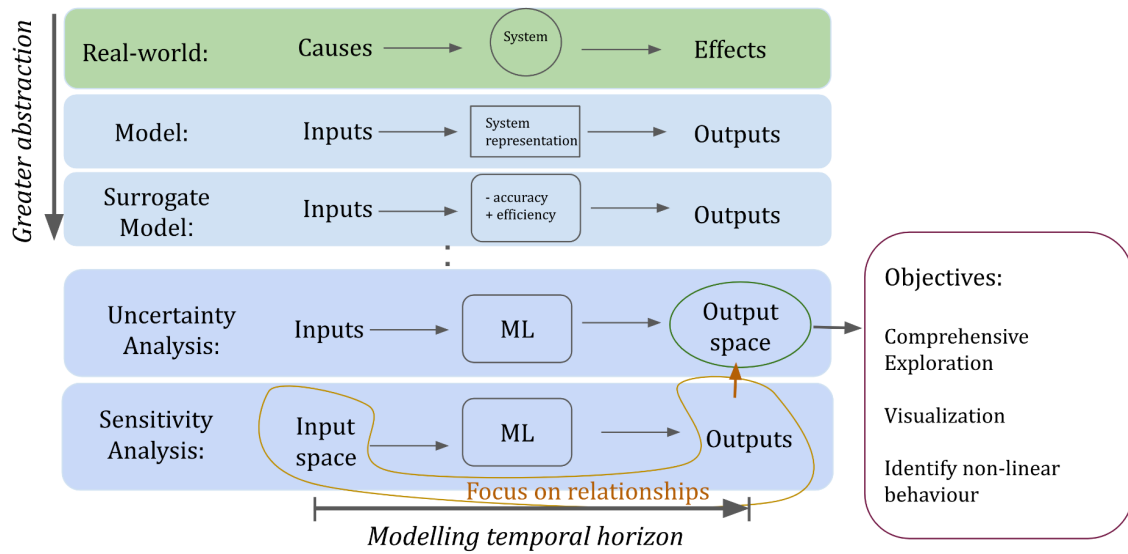


Figure 16 Real-world systems must be abstracted to produce models, introducing uncertainty, particularly where techniques are required to improve computational efficiency. While efficient models are well-suited for comprehensive uncertainty analysis, and subsequently sensitivity analysis, the associated uncertainty must be explicitly managed.

Comprehensive uncertainty analysis in energy system modeling is essential. It addresses complex problems with interconnected social, economic, and environmental relationships, like decarbonization. Uncertainty analysis improves understanding of plausible outcomes, non-intuitive behaviors, and trade-offs between objectives.

The importance of climate action highlights the need for uncertainty analysis in energy systems. Unforeseen outcomes often arise from system interdependencies, challenging expectations. For instance, increased renewable energy use may not immediately reduce emissions and could intensify land use or deplete critical materials. Quantitative models cannot always anticipate such outcomes, emphasizing the need for pluralism in modeling and analysis. Uncertainty analysis enhances exploration of possible outcomes, supporting diverse perspectives in research and decision-making [128], [129], [130].

4.2.2 Uncertainty Analysis for Power Systems

Uncertainty and sensitivity analysis are essential for modeling complex socio-technical systems. There is growing interest in standardizing their application across fields [127], [128]. Uncertainty analysis informs decision-making and policy formulation. It broadens the conceptual space, improves transparency, and promotes modeler reflexivity [127]. Power systems are highly complex due to long time horizons, significant capital investments, and interconnected social, technical, and ecological aspects. Uncertainty analysis provides insights for planning and improving system flexibility and resilience. It quantifies confidence levels within a range of plausible outcomes.

While uncertainty analysis has not been extensively applied in energy systems modelling, its importance is highlighted by the growing body of literature on the topic. For example, Gabrielli et al. [131] presented a framework for designing multi-energy systems with limited data. Their application to a Swiss urban neighborhood emphasized

the criticality of weather condition uncertainties for optimal design prioritizing cost and emission reduction. Mavromatidis et al. [132] investigated uncertainty in distributed energy systems design. Their Swiss case study revealed notable variations in the economic and carbon performance of optimal Distributed Energy Systems designs. Energy demand patterns and carrier prices emerged as significant drivers of cost variability. Aien et al. [133] provided a comprehensive review of uncertainty modelling for electric power system studies, highlighting the strengths, weaknesses, and applicability of different methods. Soroudi and Amraee [134] proposed a standard classification of uncertainty modelling techniques in energy system studies. They evaluated their strengths and weaknesses, and suggested areas for future uncertainty analysis research. Yue et al. [135] assessed uncertainty in energy system optimization models, focusing on four uncertainty approaches and their effectiveness in enhancing the policy relevance of model results. These examples demonstrate the growing relevance and importance of uncertainty analysis in energy systems modelling, despite clear gaps remaining, particularly regarding established uncertainty analysis standardization and utilization.

Uncertainty analysis in energy systems modeling, while offering valuable insights, poses computational challenges. The most prominent challenge, commonly known as the 'curse of dimensionality,' arises due to the extensive computational cost generated by the multifaceted nature of uncertainties. Adding to the complexity are non-linear relationships between input parameters and results, incorporation of real-world uncertainty, and estimation of rare events and extreme outcomes. These aspects highlight the necessity for strategies to minimize computational costs. The complexity of power systems increases the computational cost of detailed models, especially with global optimization strategies like COPPER [136]. This highlights the need for high-quality surrogate modeling techniques, such as those by Jahangiri et al. [137], to reduce computational demands while maintaining accuracy.

The complexity and computational demands of power systems modeling make traditional uncertainty analysis methods insufficient. Advanced analytical methods, such as ML, address these challenges. ML algorithms, trained on large datasets, adapt and improve over time. They replicate underlying models with greater precision and handle non-linear system aspects. ML identifies complex patterns and dependencies, providing detailed representations of system behavior.

ML plays a key role in developing surrogate models. These simplified models capture the complex relationships within energy systems while using less computational demands. ML-based surrogate models enable efficient uncertainty and sensitivity analysis. They navigate high-dimensional input spaces, examining variability and sensitivity of results. This provides a deeper understanding of system behavior across a range of scenarios and input uncertainties. ML also supports the systematic exploration of the output space, efficiently identifying key areas of interest and significant uncertainties.

ML has also been widely used for uncertainty analysis in energy systems. Gaussian process regression models have been applied to develop surrogate models of energy systems. Najibi [138] used gaussian process regression for probabilistic short-term solar photovoltaic output forecasting and decreased error by 55.5% compared to alternative

methods. Bayesian methods are another ML technique for uncertainty analysis. Zhu et al. [139] proposed a new Bayesian method to calibrate energy models of buildings. Sun et al. [140] used the Bayesian method to predict net load subject to stochasticity arising from distributed photovoltaic generation in Australia. ML models have also been deployed to manage uncertainties in energy management and planning in power systems. Aguilar et al. [141] proposed an optimization method for distributed energy resource management using ML techniques to handle uncertainty related to generation and load profiles. Results showed that the proposed scheme mostly works better than deterministic approaches in terms of penalty reduction. It demonstrated effectiveness in managing uncertainty for distributed energy resources [26] Finally, Razavi et al. [142] highlighted areas needing further focus in systems modeling. These include standardizing sensitivity analysis, addressing computational burdens, advancing sensitivity analysis in ML contexts, and clarifying its relationship with uncertainty quantification.

In summary, existing literature highlights the importance of uncertainty analysis in identifying interdependencies among energy system variables. These include generation capacity, transmission lines, load demand, and renewable energy penetration. Traditional methods, being computationally intensive, limit their usefulness for decision-makers requiring timely and accurate information. Gaps remain in applying ML to analyze complex power system design spaces with numerous input parameters and output variables. Current ML applications focus mainly on optimization and prediction. However, research on ML's exploratory use and output space correlations is limited, despite its potential to provide valuable insights into power system behavior.

This work closes that gap by utilizing Deep Neural Network (DNN) [137] as surrogate models for conventional, high-cost simulation models. This approach enables more robust uncertainty analysis in large-scale power systems. It offers a comprehensive understanding to support effective policy planning and decision-making.

Given the nonlinear nature of real-world power systems, specific analytical objectives and techniques require careful consideration. A key step is exploring the output space of power system models, covering all plausible outcomes represented by significant output variables at discrete time steps. This paper contributes to standardizing uncertainty analysis in complex socio-technical systems, extending these efforts to power systems using ML methods.

4.2.3 Contributions

This work fills that gap by introducing a novel blend of uncertainty analysis and ML in large-scale power system planning for decarbonization, addressing the notable gap in understanding the intricate interconnections and nonlinearities in system behavior over time. The originality of this paper is that it uses ML to circumvent computational limitations to characterize model behavior and explores both input and output spaces comprehensively to identify key correlations and non-linearities in system behavior, providing a more nuanced understanding essential for effective policy planning. The contributions of this work are as follows:

- **Leveraging ML for Comprehensive System Modeling:** characterizing the full scope of model behavior using ML to circumvent computational limitations.

- **Input Domain Analysis:** identifying the range, variability and uncertainty of key model inputs; including demand, capital costs, and carbon tax.
- **Output Space Variability:** identifying the range and variability of key model outputs given the uncertainty in model inputs, allowing for the variation of input parameters along multiple dimensions simultaneously.
- **Enhanced Uncertainty Analysis:** presenting and analyzing model results, plausible ranges and probability distributions to fully characterize system behavior and discuss the implications.
- **Analyzing System Behavior:** uncovering and characterizing non-linearities in the output space, regarding critical thresholds, system bifurcation, etc.

By embracing these advanced tools and methods, we aim to take the first step in revolutionizing energy systems planning, transitioning from conventional approaches to more capable, modern techniques that drive impactful advancements in the field.

4.3 Methodology

In this study, a previously developed deep learning method is utilized as a baseline to investigate the extensive design possibilities of the Canadian power system. The method [27], is employed to construct a surrogate model based on the COPPER model [143] for uncertainty analysis of the Canadian power system. The previous surrogate model's limitations are addressed by expanding the range and number of input parameters. This allows a more comprehensive examination of uncertainties in model outcomes. COPPER V7 is incorporated to overcome the constraints, storage issues, and national output limitations of COPPER V5. Transmission expansion is also included.

Once the DNN is trained, it serves as a surrogate model for COPPER in uncertainty analysis. Specifically, by providing a set of identified uncertainties in the input variables, the DNN quickly and accurately predicts the COPPER simulation for the projected state of the system. This approach enables us to explore broader pathways and conduct multidimensional sensitivity and uncertainty analyses. The surrogate model uncovers non-intuitive correlations within the design space and conduct comprehensive scenario exploration.

The ML-based surrogate model used a dataset of COPPER simulations for training. Critical uncertain inputs were identified, including carbon tax, generation type capital costs, and provincial annual demand growth rates. These parameters, with their variability, significantly influence model outputs. They serve as boundary conditions defining potential trajectories for the Canadian power sector.

To capture a comprehensive range of uncertainties related to capital costs, we expanded the existing capital cost ranges based on insights from relevant literature. We used data from six distinct sources and transformed the estimates provided by each source into equivalent annual payments over a predefined amortization period, denoted as CAD\$/kW/year, in line with the original COPPER model formulation [136], [143], [144], [145], [146], [147], [148], [149]. Next, we calculated the interquartile range (IQR) using the mean and standard deviation across all these estimates. By considering the extremes of the identified IQR and the initial range limits, as outlined in [136], we updated the range limits accordingly. In the case of battery storage, given the presence of various chemistry types,

we accounted for the capital cost associated with several chemistries, including Li-Ion (LFP), Li-Ion (NCA), Li-Ion (NMC), Vanadium flow, and ZnBr.

As per the existing policy framework [150], the current carbon pricing legislation mandates an annual price increase of \$15 per ton, starting from \$65 per ton in 2023 and reaching \$170 per ton by 2030, with no regulation beyond this date. Under the lower bound scenario, prices rise to \$95 per ton by 2025 (the base year for COPPER's carbon pricing) and then remain constant. The upper bound scenario projects prices to increase to \$95 per ton by 2025, then accelerate by \$30 per ton annually to \$245 per ton by 2030, and subsequently increase by \$20 per ton each year, reaching \$645 per ton by 2050. This modification allows the examination of the effects of both higher and lower carbon taxes on various aspects of the power system, including emissions, generation capacities, and transmission expansion.

Demand growth varies across provinces and was sourced from Canada's Energy Future Report (Canada Energy Regulator, 2023a) for 2050, using 2018 as the base year. The range was expanded by 25% on either side, a common sensitivity analysis practice. This approach captures a wider range of potential demand outcomes and accounts for variability and unpredictability in demand fluctuations [151]. The final ranges for these parameters can be found in Table 7. To ensure a comprehensive exploration of the input space, we utilized Latin-hypercube sampling (LHS) to sample these parameters across the specified ranges outlined in Table 7.

Table 7 Selected ranges for input variables based on 6 references to include uncertainties

Input variable	Range	Unit
Carbon tax in 2050	95 – 645	\$/ton
Total demand growth 2050/2018	1.2 – 2.5	Ratio
Annualized capital cost of gas combined cycle (gas CC)	106 – 198	\$/kW
Annualized capital cost of diesel	104 – 195	\$/kW
Annualized capital cost of coal	289 – 549	\$/kW
Annualized capital cost of nuclear	536 – 972	\$/kW
Annualized capital cost of biomass (waste)	285 – 574	\$/kW
Annualized capital cost of gas simple cycle (gas SC)	84 – 145	\$/kW
Annualized capital cost of wind	84 – 242	\$/kW
Annualized capital cost of solar PV	86 – 216	\$/kW
Annualized capital cost of battery storage	60 – 116	\$/kW

The COPPER model was run using these inputs, without imposing additional restrictions: constraints are not placed on national emission limit and the development of transmission, which was limited to a maximum increase of 900%.

This approach enabled the model to expand transmission within current land use and policy constraints while reducing limitations. A comprehensive range of feasible scenarios was generated. The study focuses on key national outputs for 2050, including carbon emissions, installed generation types and capacities, supply from each source, and interprovincial transmission line installations. Examining these outputs provides a holistic view of the power system's behavior.

Following data generation, the data underwent manipulation, including data cleaning, normalization, and variance clipping. Through the empirical model development procedure, the optimal hyperparameters for the model architecture were selected [143].

4.3.1 Uncertainty Analysis using Surrogate Model

To analyze model output behavior, all input parameters were populated simultaneously using Latin Hypercube Sampling (LHS) with 2000 sample points. Further sampling showed no significant changes in behavior. These samples were then supplied to the surrogate model to generate corresponding outputs, enabling comprehensive exploration of the output space.

4.3.1.1 Distribution Histograms

Histograms of output parameters show their spread by examining the shape, center, and range of distributions. These visualizations reveal the characteristics and probability distribution of each variable, including normality, skewness, and multimodality. This information supports decision-making, risk analysis, and further statistical evaluation. The histograms improve understanding of the system's potential behavior, capturing variability and uncertainty in outputs based on input uncertainties. Exploring a wide range of input scenarios provides insights into system dynamics and possible outcomes.

Measures of central tendency, such as the mean or median, provide estimates of the most probable or average output values. The spread of the distribution, indicated by the standard deviation (std) or IQR, reflects the level of variability or uncertainty in the output. Skewness measures the distribution's asymmetry, with positive skewness indicating a longer right tail and negative skewness indicating a longer left tail. Outliers or extreme values highlight potential anomalies or exceptional cases.

A concentrated distribution signifies high certainty and reliable predictions. A multimodal distribution indicates that there are several popular or common values (or ranges of values) for this parameter across different scenarios, showing system bifurcations, leading to mutually exclusive outcomes with significant policy implications. It is crucial to interpret output distributions within the context of the specific problem and analysis goals.

4.3.1.2 Quantifying Relationships in the Output Space

Investigating correlations between output variables identifies significant relationships and quantifies system tendencies as power systems evolve. These correlations offer a systems-level perspective on potential outcomes, from expected patterns to non-intuitive patterns that reveal underlying dynamics often overlooked in energy transition discussions.

To comprehensively investigate output space interdependencies and correlations, we employ two metrics. One of these metrics is the Mutual Information (MI) score, which measures the statistical dependence between two random variables. Unlike correlation, MI captures any type of statistical dependency, including non-linear and non-monotonic relationships. It quantifies the amount of information gained about one variable by observing the other,

effectively reducing uncertainty. The MI score ranges from zero (indicating independence) to larger values (signifying greater dependency). The shared information between two variables, X and Y, is defined as Eq (4) [152].

$$MI(X;Y) = \sum_X \sum_Y P(X,Y) \log \left(\frac{P(X,Y)}{P(X)P(Y)} \right) \quad (4)$$

$P(X,Y)$ is the joint probability mass function of X and Y. $P(X)$ and $P(Y)$ are the marginal probability mass functions of X and Y respectively.

Another metric used is Spearman's rank correlation coefficient. It is commonly referred to as Spearman's rho (ρ). This statistical measure assesses the strength and direction of the non-linear monotonic relationship between two variables. For a sample of size n, the n row scores X_i, Y_i are converted to ranks $R(X_i), R(Y_i)$, and r_s is computed as Eq (5) [153].

$$r_s = \rho_{R(X)R(Y)} = \frac{cov(R(X), R(Y))}{\sigma_{R(X)}\sigma_{R(Y)}} \quad (5)$$

ρ denotes the Pearson correlation coefficient, but applied to the rank variables, $cov(R(X), R(Y))$ is the covariance of the rank variables, $\sigma_{R(X)}$ and $\sigma_{R(Y)}$ are the standard deviations of the rank variables.

These metrics have their own strengths and limitations, necessitating the consideration of multiple factors for a comprehensive exploration. While Spearman's rank correlation coefficient provides information on the direction of the correlation, it cannot detect non-monotonic relationships, unlike the MI score. The combination of these metrics provides a robust means to identify associations between output variables, making minimal assumptions regarding their form.

4.3.1.3 Feature Importance Clustering

The output space comprises national outputs, which serve as the features for each of the 2000 samples in our dataset acquired from the surrogate model. To gain further insights into this dataset, we employed a technique called K-means feature importance clustering, which groups samples based on their feature values [154]. By utilizing the K-means algorithm, we identify patterns and similarities among the samples in our dataset. This approach assigns an importance factor to each output within each cluster. By extracting the most significant output variables across all groups, we understand how these variables contribute to the overall behavior of the system. This information is valuable for comprehending system behavior under different scenarios.

4.4 Results

4.4.1 Model Development

During model training, the first metric we monitor is the Mean Squared Error (MSE) loss, which indicates the accuracy of the predictions. A lower MSE loss generally suggests greater accuracy in the model's predictions. However, it is not always clear what MSE loss value should be considered a sufficiently close approximation of the base COPPER model. Prediction quality is assessed by comparing surrogate model outputs with COPPER results using the R-

squared value as a secondary metric. The R-squared value measures the goodness of fit, with 1 indicating a perfect fit and 0 indicating no fit. For each test dataset point, we calculate the R-squared value between COPPER outputs and surrogate model outputs. We then determine the minimum, maximum, and mean R-squared values across the test set. Our acceptance threshold for model performance is set at a minimum R-squared value of 0.94. The performance results, including training and test errors, are summarized in Table 8. These results indicate a high degree of accuracy in the model's predictions [137].

Table 8 Training and Test MSE losses of the model and its accuracy in predictions

Training loss (MSE)	Test loss (MSE)	Mean (R^2)	Std (R^2)
0.0039	0.01	0.96	0.020

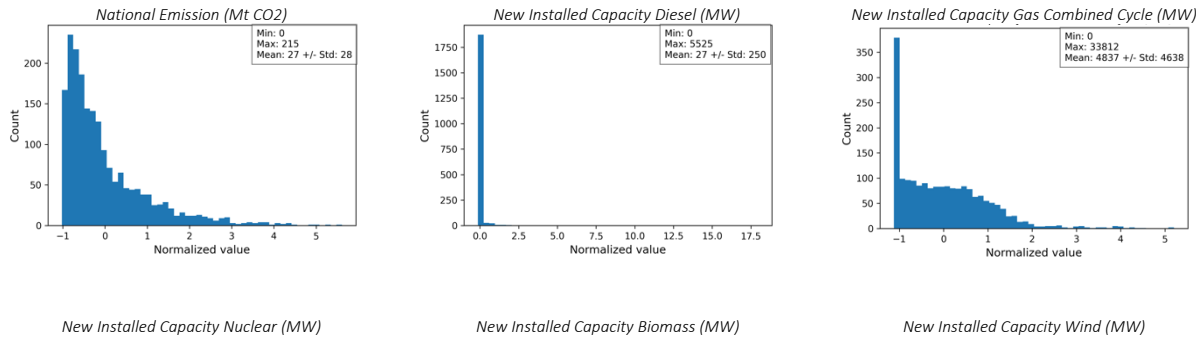
Table 10 compares the proposed model's run-time and resource use with COPPER. It shows significant reduce in computational costs and resource requirements. This enhanced efficiency enables more feasible scenario exploration without specific computational constraints.

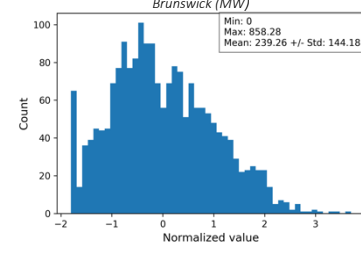
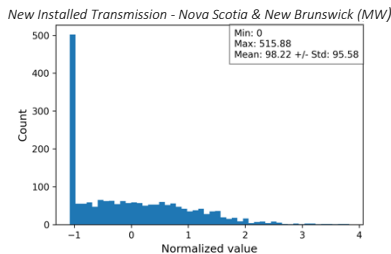
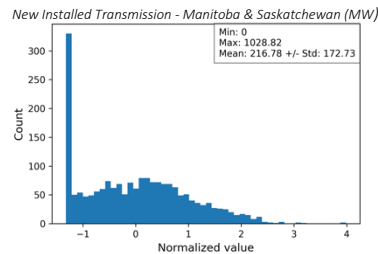
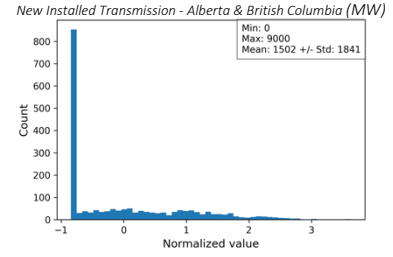
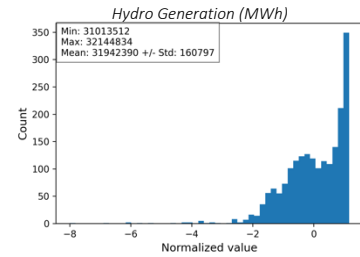
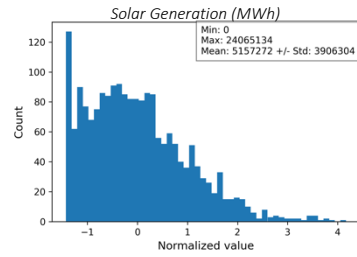
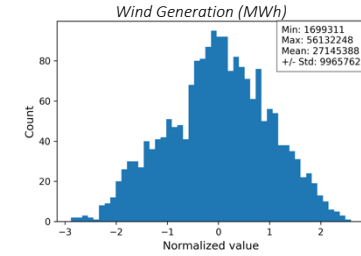
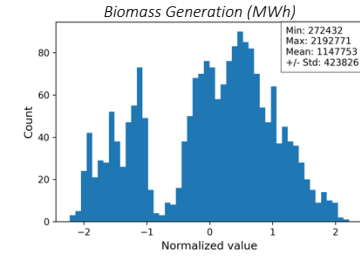
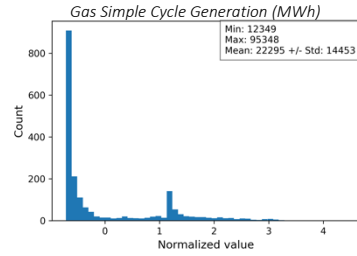
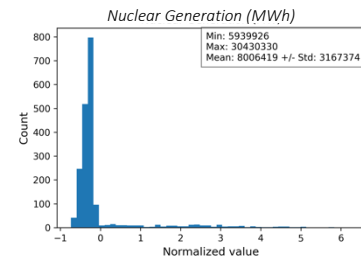
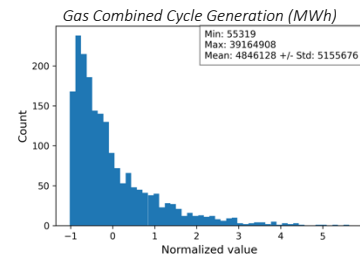
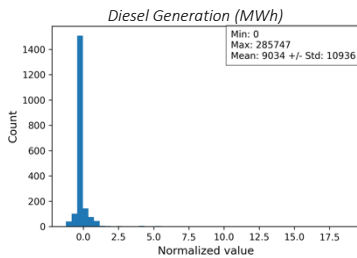
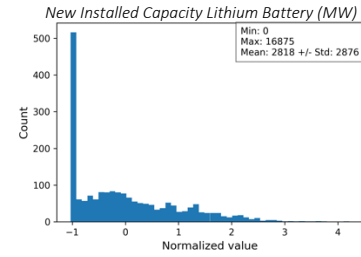
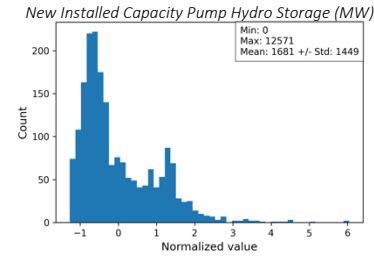
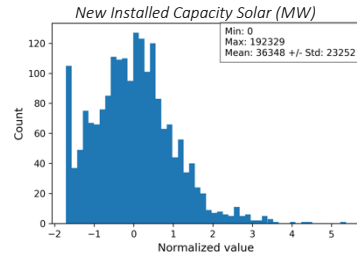
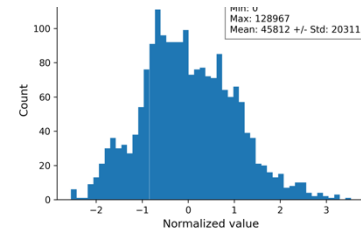
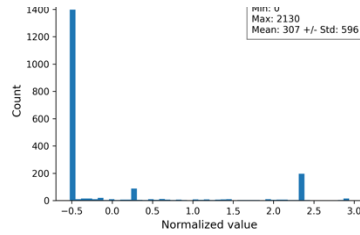
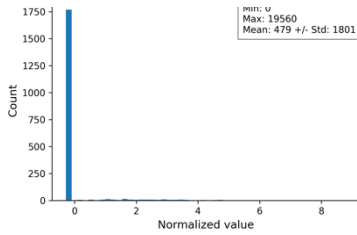
Table 9 Comparison of COPPER and the proposed model computational costs and run time

Model	CPU	Memory	Run-time
COPPER	16 - 32	64 - 128 GB	15h - 72h
Residual neural network	1	1.5 MB	10 milliseconds

4.4.2 Uncertainty Analysis

Histograms of output distributions provide high-level insights on the outputs behavior by presenting their range and tendencies. The output statistics in Figure 17 provide a snapshot of future scenarios for the power system. They support planning for sustainable power infrastructure. The distribution plots of output variables are categorized as multimodal, centrally or extremely spread, unimodal, and largely non-stochastic.





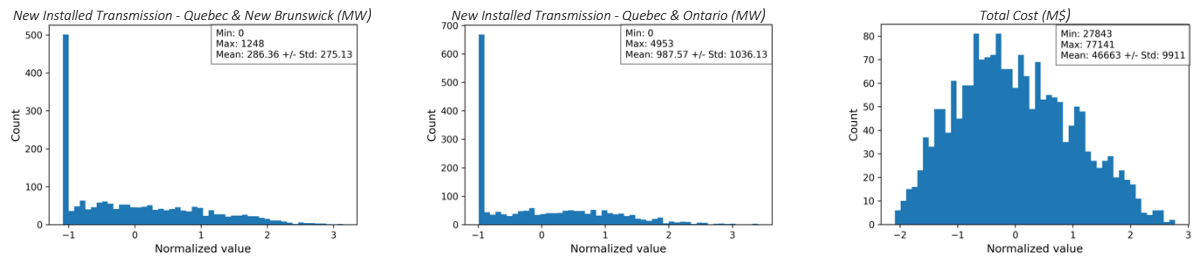


Figure 17 Distribution of projected output variables of the Canadian power system in 2050 (Negative bins do not mean negative values of variables, they show values lower than average)

Figure 18 and Figure 19 exhibit the MI score and Spearman's rank values respectively for variables within the Canadian power system (the non-stochastic variables in the histograms are removed from the exploration of interdependence).

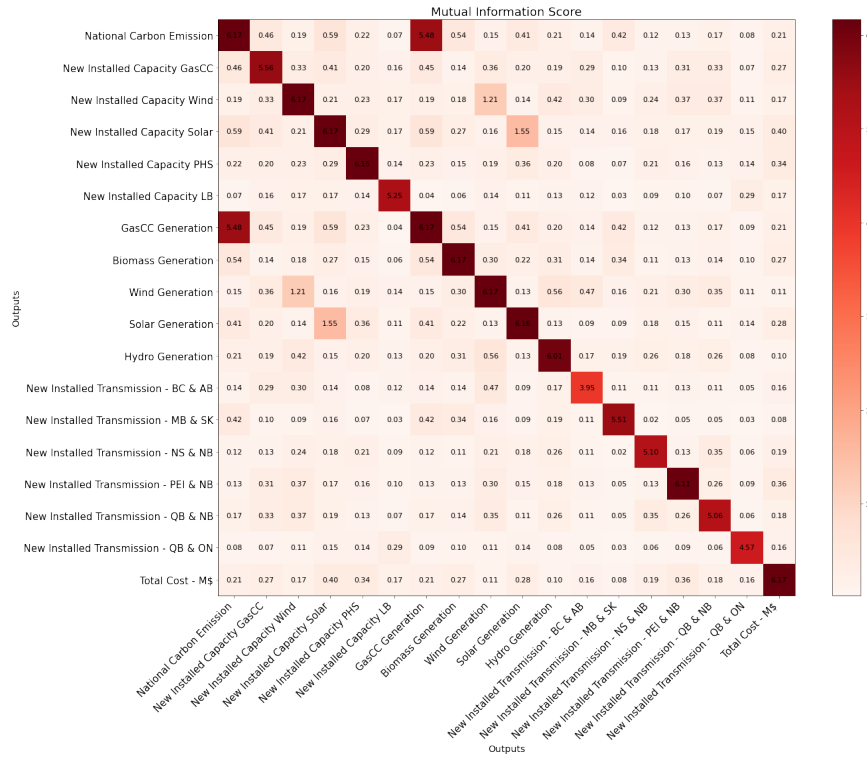


Figure 18 MI score values between output variables of the Canadian power system in 2050

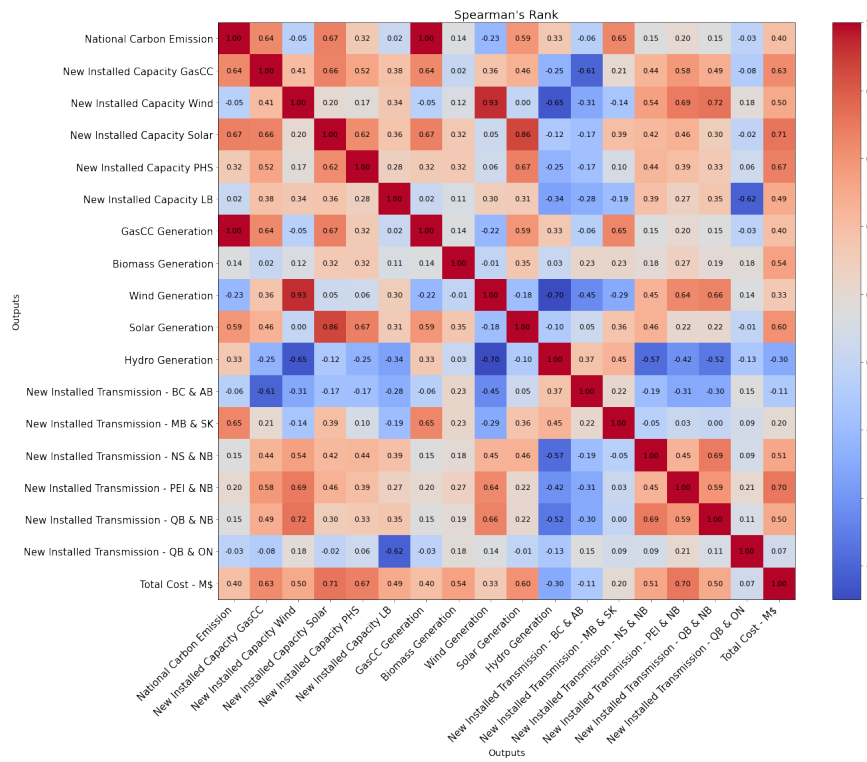


Figure 19 Spearman's rank values between output variables of the Canadian power system in 2050

Key outputs influencing scenario differences and diverse pathways are analyzed using feature importance clustering. The silhouette score [155] is used as a metric to identify the optimal number of clusters. A higher silhouette score, closer to one, indicates a more cohesive clustering arrangement. Accordingly, we determine that 16 clusters align with the maximum silhouette score. Figure 20 depicts a bar chart of the importance values for each output in clustering. Higher weights indicate higher deterministic outputs in clustering and consequently shaping different pathways.

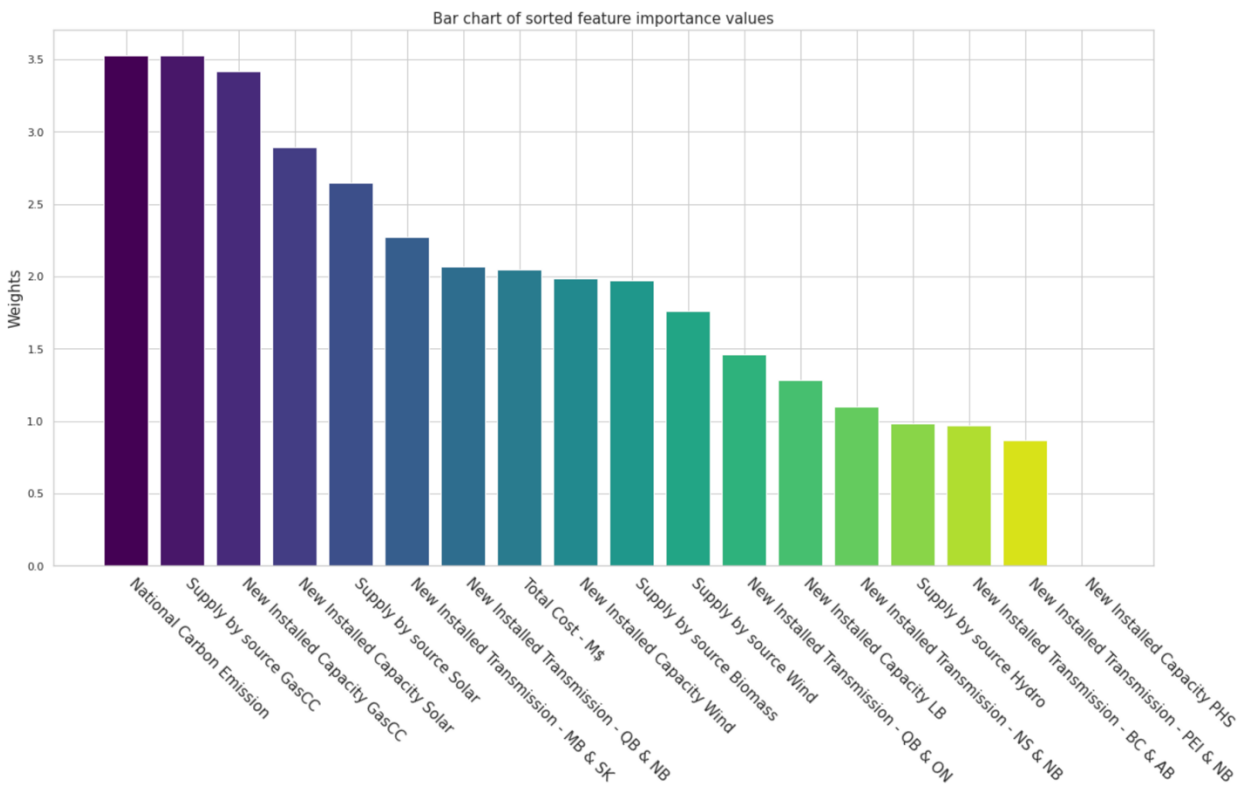


Figure 20 Importance Weight of output variables in clustering

The following section presents insights derived from histogram distributions, correlation heatmaps, and clustering results.

4.4.2.1 Technologies with Robust Evolution

The evolution of several technology types remains robust against a breadth of input assumptions. Certain variables exhibited distributions with considerable spread around central or extreme values, suggesting a wide range of plausible output. This kind of distribution implies that there is a robust pathway for a specific generation technology. Varying inputs does change the trajectory of that technology but around the central pathway. The central tendency indicates the "typical" or most likely level of that output. Extremal tendencies, on the other hand, represent the potential maximum and minimum output. These variables include national carbon emission, total cost, new installed capacity, and generation of solar and wind, new installed transmission of Prince Edward Island-New Brunswick, and

new installed capacity and generation of gas combined cycle (gas CC). We delve into detail for some of the more significant points:

A spread in the distribution suggests variability in the gas CC's generation (min 55.3 GWh, Max 39.1 TWh, mean 4.8 TWh, std 5.1 TWh) and new installed capacity (min 0, Max 33.8 GW, mean 4.8 GW, std 4.6 GW). The extremal tendency represents potential maximum or minimum outputs. It reflects the plant's capacity to ramp up during peak demand or scale down when other resources are plentiful. Gas CC positively correlates with both solar and wind, implying that these generation types might be used in tandem to balance the intermittent nature of renewable energy.

A wide distribution with both central and extremal tendencies for solar generation (min 0, Max 24 TWh, mean 5.1 TWh, std 3.9 TWh) and new installations (min 0, Max 192 GW, mean 36 GW, std 23 GW) indicates a wide range of plausible scenarios, from moderate to extreme. The central tendency shows scenarios where solar generation and capacity installations align with the average, reflecting typical conditions. The extremal tendency indicates cases where solar generation and installations could be significantly above or below average. These extreme events are rare, occurring under limited input combinations. Solar generally follows the central trend, suggesting a robust pathway.

The role of solar in differentiating various scenarios is discovered to be more significant than that of wind. This observation aligns with the unique distribution patterns of solar outputs, unlike wind which exhibits only central tendencies. The presence of these dual tendencies in solar indicates its significant influence on decision-making and strategy formulation.

A wider distribution of wind compared to solar implies that wind generation (min 1.6 TWh, Max 56.1 TWh, mean 27.1 TWh, std 9.9 TWh) and new installation (min 0, Max 128.9 GW, mean 45.8 GW, std 20 GW) have even more variability. The high central tendencies show the most likely outcomes (~ 68%) are concentrated around the average scenario and implies a significant role for wind power in the energy mix. This is because wind capacities are studied to have a pivotal role in the decarbonization pathways of the Canadian power system.

The spread distribution of solar and wind generation and new installed capacity highlight both the potential and the challenges of renewable energy in the Canadian power system. A high central tendency for both wind and solar generation implies a significant contribution from these zero-emission sources. This is a positive sign for decarbonization efforts.

The costs for wind and solar comprise capital costs, and transmission expansion costs based on the locations' distance to the closest bus. Expanding the wind and solar capacities depends on varying capacity factors and their locations for distance and capacity factor considerations. Wind and solar capacity expansion show more non-linear patterns in the output space. Multiple modes in their distributions indicate bifurcations and discontinuities. Generation is influenced by demand and capacity factors. Comparing wind and solar installed capacity with generation plots shows discrepancies, highlighting the importance of capacity factors. Additionally, wind generation

is less correlated to the installed wind compared to the same couple of variables in solar. This is because building more wind capacity means moving to locations with a lower capacity factor. In the meantime, solar capacity factors for solar are more uniform in different grid locations.

4.4.2.2 *Hydro Power's Persistent Significance Across Input Assumptions*

It appears that hydro generation (min 31 TWh, Max 32.1 TWh, mean 31.9 TWh, std 0.1 TWh) tends to lean towards the higher end (~ 42.5 % of scenarios), indicating that hydro generation is less sensitive to inputs. Hydroelectric power has an essential role in fulfilling energy demand. It is valuable for its flexibility and cost-effectiveness. Hydropower accounts for 60% of the total electricity production in Canada, underlining its substantial contribution to the energy system. This contribution is expected to remain significant until 2050 due to the continued operation of existing hydroelectric facilities.

The correlation between hydro and wind output is observed to be negative. As a result of expanded wind capacities, output from hydro, which serves as a flexible power source, is likely to decrease in order to integrate increased, cheaper electricity generation from wind power.

The total cost of the system is positively influenced by all new build generation types except hydro. The reason is that hydro is not expanding. Additionally, hydro generation ranks among the least deterministic variables in power system scenarios in clustering results, due to its relatively stable, and less variable nature.

4.4.2.3 *Bifurcation in the Gas SC Generation*

Certain variables display multimodal distributions including gas SC generation (min 12.3 GWh, Max 95.3 GWh, mean 22.3 GWh, std 14.4 GWh) and biomass generation (min 272.4 GWh, Max 2.1 TWh, mean 1.1 TWh, std 0.4 TWh). The multimodal distribution of gas SC generation indicates multiple possible configurations. These depend on input parameter settings, including carbon tax variability. This multimodal distribution reveals important information:

Peaks in gas SC generation occur when low-carbon sources are limited or demand is high, requiring gas peaking plants to meet the load. This indicates the need for more renewable generation, storage, or demand response measures to reduce the need for gas SC during these times. Correlations between outputs reveal such instances in low carbon tax scenarios. Emission-intensive plants, like gas SC, generate low-cost electricity in these cases.

Peaks with low gas SC generation occur when the grid can meet its needs with less carbon-intensive resources. Studying these scenarios provide insights into the conditions that allow for lower gas use, such as high renewable availability or low demand. These instances occur in high carbon tax rates, which limit generation from such plants.

The multimodal distribution of gas SC generation reflects its complex role in the Canadian power system. Gas SC generation comes from existing assets, with no new capacity installed across the output space.

4.4.2.4 *Dominant Technologies in the Least-cost Decarbonized Pathways*

Some variables exhibited unimodal distributions with slight skewness. These distributions suggest a dominant outcome with variations around it. Variables in this category include new installed capacity of lithium battery (LB)

(min 0: ~25% of scenarios, Max 16.8 GW, mean 2.8 GW, std 2.8 GW), new installed transmission of British Columbia-Alberta, Quebec -Ontario, and Quebec-New Brunswick.

The unimodal distribution of new installed LB storage capacity suggests a common strategy for its use. This reflects its role in balancing renewable energy intermittency. The skewness toward the lower end suggests COPPER addresses flexibility for wind and solar integration using other resources. These include PHS and flexible generation types like hydro and gas CC.

4.4.2.5 *Interprovincial Transmissions in the Decarbonization Pathways*

Unimodal distributions are observed for new installed transmission of British Columbia-Alberta (min 0: ~ 42%, Max 9 GW, mean 1.5 GW, std 1.8 GW), Quebec-Ontario (min 0: ~34% of scenarios, Max 4.9 GW, mean 0.9 GW, std 1 GW), Quebec-New Brunswick (min 0: ~25% of scenarios, Max 1.2 GW, mean 0.2 GW, std 0.2 GW), and Manitoba-Saskatchewan (min 0: ~17% of scenarios, Max 1 GW, mean 0.2 GW, std 0.1 GW). These variables imply a typical pattern for new transmission installations across these provinces. Transmission capacity expansion is driven by accessing regions with higher Variable Renewable Energy (VRE) potential.

This strategy prompts the model to build wind or solar capacity in optimal locations and use transmission lines to distribute power to neighboring provinces. The correlation between VRE capacities and transmission expansions in high-potential provinces, such as Alberta, Saskatchewan, Quebec, and Ontario, supports this behavior. However, for some interconnections, this behavior may not be as predictable. Limited load growth, as seen in New Brunswick, or similar VRE potentials between provinces reduces the robustness of transmission capacity expansion.

There appears to be a significant co-occurrence of eastern grid expansions, specifically between Quebec-New Brunswick and Nova Scotia-New Brunswick (min 0: ~25% of scenarios, Max 515.8 GW, mean 0.9 GW, std 0.9 GW). When one expansion occurs, the other is likely to follow. Increasing transmission capacity in one region may require upgrades in neighboring areas to manage higher electricity flow.

Minimal correlation between certain outputs, like new transmission between provinces and new LB and PHS capacity, suggests independent behavior. This means that changes in the new transmission capacity of Quebec-Ontario, for instance, do not significantly impact changes in the new transmission capacity of British Columbia-Alberta. Similarly, the decision to install new LB or PHS capacity appears to be independent of the installation of these transmission lines. These low correlations suggest that planning and investment decisions in these specific areas can be made with more flexibility and independence. However, the lack of correlation might also point to potential opportunities for more coordinated planning to maximize system efficiency and resilience.

Eastern grid expansion increases all generation sources except hydro. Existing hydro resources remain active without expansion, while other generation capacities tend to grow. Total cost is positively influenced by all transmission lines except with British Columbia-Alberta transmission. The reason is that British Columbia - Alberta transmission is relatively cheap.

New transmission lines between Manitoba-Saskatchewan and Quebec-New Brunswick show the most influence on scenario differences. Their variability highlights a pivotal role in power system planning and management. In contrast, Prince Edward Island-New Brunswick (min 0, Max 0.8 GW, mean 0.2 GW, std 0.1 GW) and British Columbia-Alberta demonstrate lesser determinism. The distinction arises from stronger correlations in the former transmission lines and weaker correlations in the latter, as shown by correlation metrics.

Transmission Expansion and VREs. Transmission between western provinces, particularly British Columbia-Alberta and Saskatchewan-Manitoba, influences power generation patterns. Correlations exist between wind and gas CC for British Columbia-Alberta and between gas CC and biomass for Saskatchewan-Manitoba.

In the eastern grid, similar dynamics occur. Transmission expansion, especially Quebec-New Brunswick and Quebec-Prince Edward Island, influences generation choices, particularly between gas CC and wind.

Transmission build between Quebec-Ontario primarily affects LB build. This is attributed to access to Quebec's hydro resources, potentially reducing the need for extensive energy storage.

Wind supply is strongly correlated with Alberta- British Columbia corridor expansion. Interestingly, the corridor plays a crucial role in providing access to Alberta's high wind potential locations, and British Columbia's flexible hydro capacities.

These observations show strong correlations between VRE and transmission expansion across provinces. VRE capacity factors drive these correlations by encouraging expansion in higher-potential locations. Based on that, the model decides to build more wind/solar in one location with more potential and transfer it to neighboring provinces. Canada's power system decarbonization relies on accessing high VRE regions. Generation is distributed across the country using transmission. Hydro provides backup. The VRE capacity factor limitation for transmission will impact gas CC generation choices as the non-renewable energy source. Similarly, a correlation between gas CC and solar power generation is observed. It suggests these generation types often be used in combination within the power system.

4.4.2.6 Uncertainty in the Future Trajectory of Storage Assets

A multimodal distribution with a left extremal tendency for new installed capacity of pump hydro storage (PHS) (min 0, Max 12.5 GW, mean 1.6 GW, std 1.4 GW) reflects various potential operational scenarios or strategies. The left extremal tendency (~ 45% of scenarios) suggests that there are cases where significantly less new PHS capacity is installed than average, indicating scenarios where other types of storage or generation options may be more optimal. This shows the importance of considering a diverse set of options in the planning and optimization of energy systems. It is also indicating that there is still a lot of uncertainty in the future of storage in power systems.

New LB and PHS installations correlate with gas CC, solar, and wind. These storage technologies are often built with these generation sources. They help balance output and ensure grid reliability. Gas CC is another flexible capacity to support the requirements to integrate larger wind and solar capacities at lower carbon tax rates.

The installed capacity of LB influences scenarios more than PHS. This doesn't affect COPPER model pathways and outputs. Cost uncertainty drives this impact.

4.4.2.7 Exclusion of Nuclear and Diesel Generation in the Future Grid Development

Nuclear (min 5.9 TWh, Max 30.4 TWh, mean 8 TWh, std 3.1 TWh), in ~85% of scenarios and diesel, in ~ 72% of scenarios, are not built or generated in most future grids. Furthermore, generation and expansion outputs stay within a small range. These variables show non-stochastic behavior. It shows outputs are less influenced by input variations. Nuclear is not sensitive, as its capital cost is much higher than other resources, thus, the model does not build it in many cases. Nuclear energy supports decarbonization with zero emissions. Its predictability helps long-term planning and grid stability. Diesel is an emission intense resource. It is most likely that the model doesn't build out any diesel in most of the carbon taxation inputs.

4.4.2.8 Drivers for Carbon Emissions

Spread distribution of national carbon emissions reflects the inherent variability of this output variables. This is because of the wide range of carbon tax policy affecting the emission.

Carbon emissions have a strong association with gas CC. After gas CC, solar, biomass, and installed transmission of Manitoba-Saskatchewan affect national emissions the most. This highlights these factors as key contributors to the system's carbon footprint. While gas SC mainly plays as a peaking capacity in higher carbon tax rates, gas CC remains the main contributor to emissions in lack of other emitting sources which retired due to high emission rates and carbon taxation. These correlations help in identifying the most effective strategies for emissions reduction. If certain renewables, solar and biomass, or transmission enhancements of Manitoba-Saskatchewan are more strongly correlated with emission reductions than others, these might be prioritized in future system development or policy efforts.

4.4.2.9 Factors Shaping Divergence in the Energy Transition Pathways

The carbon emission levels, generation and the new installed capacity of gas CC, with the maximum feature importance weight (~ 3.5), and solar power systems, (feature importance weight 2.8) have the most influence on creating diverse scenarios within the Canadian power system in 2050. These factors play a pivotal role in shaping the various pathways and outcomes observed in the different scenarios.

Notably, all these output variables are among the most correlated outputs based on the correlation metrics values presented in heatmaps. The reason is that stronger correlations indicate a greater number of variables influencing a specific output. This influences more output variables and shaping diverse scenarios. This introduces more variations and uncertainties. Therefore, these variables are more influential in the planning of different energy pathways and demand careful consideration.

4.5 Limitations

Like all modeling methods, our approach also has limitations from two sources: the COPPER model and the ML surrogate, beyond those in past studies [136], [143].

Firstly, the COPPER model uses a fixed capacity factor. It ignores capacity transfers, like building a plant in one area and selling capacity elsewhere. The model's focus is primarily on energy transfer, resulting in capacity for transmission construction that is majorly driven by the availability of VRE potentials. COPPER also simplifies assumptions by treating transmission and most generation technologies as continuous variables rather than binary integers. A realistic approach models projects with known capacities. Regional analysis could reduce computation. Additionally, COPPER ignores landscape factors affecting wind and solar. It may overstate potential in some regions. Balancing areas and intraprovincial transmission are limited [12].

Secondly, the limitations related to the ML surrogate pertain to its dependence on the current COPPER version. As COPPER evolves, retraining the surrogate model ensures changes are captured and integrated. The reliability of the surrogate model depends on the quality and comprehensiveness of the training data, with potential inaccuracies when extrapolating beyond the training data. The ML model also exhibit less sensitivity to parameters with small nominal values, potentially affecting predictive accuracy for certain provinces. Finally, while the surrogate model provides predictive power, understanding the specific reasons behind its predictions can be challenging, impacting interpretability [156].

4.6 Discussion

This paper advances large-scale power system planning. It applies ML methods to overcome computational limits of conventional models for uncertainty analysis. The existing literature primarily focuses on utilizing ML for predictions and optimization in various fields. While there are studies that examine uncertainty analysis using ML to estimate prediction errors, there is a noticeable lack of research on standardized uncertainty analysis. Specially, by exploring the output space of large-scale power systems. The focus of uncertainty analysis is not on prediction, but on exploring and characterizing the output space. By understanding the behavior of the system through analyzing results probabilistically, considering input uncertainty, and exploring correlations among outputs. This probabilistic analysis provides insights into system behavior and its implications and enables the exploration of key output variability. Additionally, the exploration of output correlations uncovers relationships and dependencies among variables, enriching the understanding of complex system interactions. This holistic approach enhances decision-making capabilities and facilitates predictions under various scenarios. It contributes to a comprehensive characterization of model behavior.

Exploring output interdependencies lead to more effective power system planning. For example, understanding the least correlated variables help identify areas of independent planning or where there are opportunities for improved coordination. On the other hand, knowledge of the most correlated variables helps predict system-wide impacts. It supports integrated, sustainable planning decisions. In terms of decarbonization, recognizing the variables that correlate strongly with national carbon emissions guide strategies to reduce these emissions.

Lastly, the presence of some non-intuitive correlations among the output variables can be attributed to the underlying demand growth, indicating that demand-side factors influence these relationships. The observed

correlations primarily stem from the stochastic demand as an input, rather than indicating direct relationships. While further investigation into this matter is beyond the scope of this discussion.

4.7 Conclusion

This study emphasizes the importance of uncertainty analysis in energy systems, particularly in large-scale power systems, and highlights the limitations of traditional methods. The research identifies gaps in applying ML to analyze complex power systems and calls for exploratory ML approaches to gain valuable insights. The use of neural networks as surrogate models is proposed to enhance uncertainty analysis and inform policy planning. The paper standardizes uncertainty analysis in power systems. It extends ML methods for input and output exploration. This addresses research gaps and explores output correlations for better decision-making. This study brings a new perspective to power system modeling, offering valuable insights into system behavior, causative factors, and distinct decarbonization pathways. The most important takeaways of this study are:

- Further research is needed on capacity factor uncertainties. They significantly impact power system outcomes.
- Gas CC power (generation mean 4.8 TWh, installed capacity mean 4.8 GW) emerged as a more flexible option than gas SC (generation mean 22.3 GWh 0 installed capacity), showing a lower impact from carbon taxation due to its lower emission factor. While gas CC is less impacted by carbon tax, it is utilized in the model to support large wind and solar integration even at very high tax rates. While the emissions are low in this technology, deep decarbonization of the power systems dictates other policies in addition to carbon taxation.
- Hydroelectric power, a key part of Canada's energy mix, showed low sensitivity to input changes. It stayed stable (in ~42.5% of scenarios). It will support large VRE integration and power system decarbonization. However, its expansion is less impacted by the selected input parameters and their range. Hydroelectric remains important but must be maintained and developed in a new way that respects the very legitimate concerns that currently face it i.e., disclosure of Site C dam.
- Transmission expansion patterns reflect the influence of VRE capacity factors and their difference in different locations. Correlations, like that between Alberta's wind potential and the Alberta- British Columbia line, reinforce this point. The VRE capacity factor limitations also had ripple effects on non-renewable source choices, favoring combinations like gas CC with wind and solar. This insight also emphasizes the importance of transmission expansion and power systems integration in the decarbonization pathways.
- Nuclear and diesel powers respectively in ~ 85% and ~ 72% of scenarios, owing to their high cost and emission respectively, were less favored. They emerged as almost non-stochastic variables. With no cap on emissions, these two technologies are not selected to provide firm capacities even in higher wind and

solar penetration rates. As such, nuclear is not selected over gas CC even in the lower capital cost inputs. Diesel capacities remain unused even with low carbon taxes. Policymakers should avoid relying on nuclear and diesel. Deep decarbonization needs strong regulations alongside carbon taxes.

- Carbon emissions, gas CC and solar powers are key differentiators in future power system scenarios. Solar held a more significant role than wind in these differentiations. For storage, the installed capacity of LB was more influential than PHS. While in transmission lines, Manitoba-Saskatchewan and Quebec-New Brunswick had the most and Prince Edward Island-New Brunswick and had British Columbia-Alberta the least influence. These insights provide guidance for policymakers, highlighting the key areas that require attention for effective planning and decision-making.
- Further research investment is needed to better understand and forecast demand, as it drives pathways, contributes to non-intuitive correlations, and remains uncertain.

The findings developed using ML and numerical analysis have potential implications that can be further explored in future research. This includes incorporating uncertainties associated with wind and solar capacity factors to refine power system modelling. Furthermore, a provincial-level application of the methodologies developed in this study could lead to more tailored insights for effective provincial policy planning. In considering future research directions, it's essential to acknowledge additional factors that may influence power system modeling accuracy and policy planning outcomes. For instance, variations in the quality of wind and solar resources, distance to load centers, landscape characteristics, and interprovincial transmission costs can significantly impact grid decarbonization strategies. While current methodologies like COPPER accurately quantify resource quality and transmission costs, there's potential to explore the effects of land availability and interprovincial transmission capital costs on decarbonization efforts further. Addressing these factors presents an opportunity to refine modeling techniques and develop more tailored policy interventions. However, challenges persist in validating data accuracy, managing computational demands, and ensuring model scalability.

4.8 Author Contributions

Zahra Jahangiri: contributed to conceptualization, methodology, software, validation, formal analysis, investigation, writing (original draft), and visualization, **Mohammad Miri:** contributed to conceptualization, and writing (reviewing), **Kwang Moo Yi:** contributed to supervision, resources, writing (reviewing), **Madeleine McPherson:** contributed to supervision, resources, writing (reviewing and editing), and funding acquisition.

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5 Chapter 5: A Machine Learning Approach to Analysis of Canadian Provincial Power System Decarbonization

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5.1 Abstract

Canada committed to reducing national greenhouse gas emissions by 40-45% by 2030 and achieving net-zero by 2050. It relies on low-carbon electrification across economic sectors. This study explores machine learning's potential for least-cost optimization of Canadian provincial power systems to 2050. It identifies robust pathways for net-zero emissions and provides policy insights on wind, solar, gas emissions, and interprovincial transmission expansion. Surrogate modeling tests sensitivities to capital costs, electricity demand, and carbon pricing using results from a capacity expansion model. Under almost all future scenarios, six provinces develop new wind generation, with substantial deployment in Alberta (mean 27.3 GW, max. 62.7 GW), Ontario (mean 6.8 GW, max. 19.3 GW), Saskatchewan (mean 3.6 GW, max 8.9 GW) and Manitoba (mean 1.5 GW, max 3.5 GW). With the potential exception of BC, where higher-cost wind generation results in solar generation becoming the primary low-carbon electrical energy source (mean 25.2 GW). Future solar generation across Canada is more limited (mean 37.1 GW) and less certain than wind generation in all other Canadian provinces. Existing natural gas generation is maintained in almost all scenarios in all provinces. It provides support for maintaining these resources for reliability and reserve requirements. Very limited natural gas is developed under any scenarios, with the exception of BC (mean 4.3 GW) where more than 80% of scenarios include new natural gas capacity. Additional transmission transfer capacity is developed in most scenarios between BC-Alberta (~60% of scenarios), Saskatchewan-Manitoba (~85%), and Ontario-Quebec (~75%). Carbon prices, along with wind and solar capital costs, act as primary determinants of least-cost decarbonization pathways. These findings offer insights for Canadian policymakers into net-zero pathways for provincial electricity systems that remain robust despite variability in inputs.

Key words: *Provincial Policy Planning, Decarbonization Pathways, Energy Systems Modeling, Machine Learning*

5.2 Introduction and Motivation

As a party to the Paris Agreement, Canada committed to reducing national economy-wide greenhouse gas emissions (GHG) by 40-45% by 2030 [157] and to net-zero by 2050 [158]. Achievement depends on electrification, generation decarbonization, and technology evolution [44], [12]. Decarbonization studies of Canada's electricity sector show large hydro, wind, or nuclear buildouts [42], [43], [12]. Some scenarios also show significant transmission expansions [159]. These studies explore technically or economically viable national strategies. This approach struggles to find robust decarbonization pathways due to policy uncertainties and model limits.

Electricity in Canada is provincially regulated. Meeting national emissions targets requires addressing provincial economies [13], geographies, technology costs, and policy [14]. Canadian provincial economies differ substantially in their sectoral contributions to gross domestic product (GDP) and in their per capita GDP (Figure 21). Contributions of the energy sector (i.e., oil, natural gas and coal production and distribution) to GDP range from a fraction (1.2% in PE) to nearly a quarter (23.0% in AB) of provincial economies. They contribute proportionately to provincial emissions and substantially (28.2%) to national emissions [160]. The range in per capita GDP (~\$42k in the Maritimes to ~72k in Alberta) reflects differences in consumer ability to finance the costs of electricity decarbonization [39], [40]. Some Canadian provinces have abundant variable renewable, hydroelectric, or nuclear generation while others rely heavily on fossil fuels. It results in electricity sector GHG emissions intensities ranging from 1 to 670 tCO₂e/GWh [15] (Figure 22). Some regions face development limits or lack low-carbon resources for renewables (e.g., storage hydroelectric). Others lack quality storage sites or need transmission expansion. These factors drive variability in decarbonization costs. [161].

Notwithstanding provincial regulation of the electricity sector, Canadian provinces are subject to federal regulations supporting national decarbonization efforts [21].

These include economy-wide carbon pricing with an output-based pricing system (OBPS) to protect competitiveness [16], [17], [18], phasing out coal-fired generation by 2030 [19], and setting performance standards (370 tCO₂e/GWh) for gas-fired generation [20]. In addition, to limit remaining emissions from natural gas generation beyond 2030 [12], pending regulations require net-zero provincial electricity systems by 2035 [22].

Provinces phasing out fossil fuels, adopting renewable standards, and using feed-in tariffs reduce electricity emissions. Federal and provincial policy misalignment could limit national reductions [11].

Some provinces prohibit nuclear or large hydro development [162], [163]. Renewable energy and GHG reduction targets differ across provinces. Provincial carbon pricing regimes also vary despite the federal carbon pricing mechanism [164]. Recent studies also indicate that least-cost decarbonization in some provinces entails development of inter-provincial [23], [24] and international transmission [24], [25]. Multi-year federal efforts to expand regional transmission in Atlantic Canada ended [26]. Provincial utilities chose a modest expansion of an existing transmission link [27]. Provincial analyses can give planners deeper insight into challenges and opportunities. They can also inform policies on renewables, gas emission reduction, and transmission expansion.

The focus on pathway analysis leads to electricity modeling based on least-cost optimization, simulation, and single-factor sensitivity. This conventional approach limits net-zero pathway evaluation. Robust analysis needs a broad review of strategies and technologies under power system uncertainties. First, conventional approaches are computationally intensive, limiting available scenarios for exploring sensitivities associated with alternative futures. Secondly, these approaches typically assume deterministic relationships between variable inputs and model outputs, limiting their application for decision-making under uncertainty. Power systems are subject to significant

variability in technology costs, operations, policy constraints, and future electricity requirements, particularly on the multi-decadal horizon of deep decarbonization. Thirdly, conventional models often ignore correlations between parameters and inputs. These correlations can reveal cost-effective, lower-risk decarbonization opportunities for policy decisions.

Machine learning (ML) models offer a potential solution to charting decarbonization of Canadian provincial electricity systems while accounting for uncertainties and variabilities. A recent review of ML techniques demonstrated increased interest in using ML to address technical challenges in evolving power systems [47]. These challenges in forecasting renewable energy generation and future deployment stem from multifaceted uncertainties inherent to wind [165] and solar [166] resources and to evolution of technologies [167] and costs [168]. These uncertainties involve complex non-linear relationships between input parameters and outcomes, and the integration of real-world uncertainties into modeling frameworks. Estimating rare events and extreme outcomes poses additional challenges due to their infrequency and impact. Moreover, long-term electricity planning and interlinked socio-technical factors increase uncertainty. This is especially true in detailed modeling of optimization strategies.

By capturing complex correlations and relationships between model parameters and input variables, ML models account for uncertainty and variability in wind and solar generation [169] and power system evolution [46]. It supports more robust decarbonization strategies that are optimal or near optimal under a wide variety of future conditions. With large datasets from multi-factor uncertainty, ML models can learn patterns and relationships not visible to conventional models [170]. An exploration of ML techniques in power systems highlighted advantages and limitations compared to conventional techniques. It concluded that ML offers significant potential for real-time applications in power systems [48]. ML methods have been applied to load forecasting and power system optimization problems [49], to determining the importance of stakeholder and planning criteria in system expansion planning [50], and to solving complex control problems in power systems [9]. A recent analysis used ML with principal component analysis and clustering. It identified representative days for a reduced capacity expansion model on grid decarbonization [10].

These investigations demonstrate the potential of ML models to improve the accuracy and efficiency of power system planning and modeling. However, none of these studies explore the potential of ML in capacity expansion models to explore correlations, uncertainties, and variability in different input parameters affecting power system evolution. Exploiting the capabilities of ML methods in capacity expansion planning could improve policymaking and planning for decarbonizing these regional electricity systems [137].

Contributions. Our contributions to energy systems modeling using ML models are as follows:

- Providing insights into least-cost pathways to net-zero electricity system decarbonization that remain robust despite technology and policy uncertainties and variabilities. The goal is informing effective policy, planning and decision-making for provincial grid decarbonization in Canada.
- Investigating ML models for least-cost optimization of provincial power systems. The focus is on net-zero emissions under uncertainties in costs, demand, and carbon pricing.

- Using ML methods to analyze power system uncertainty and variability. This approach reduces computational costs.

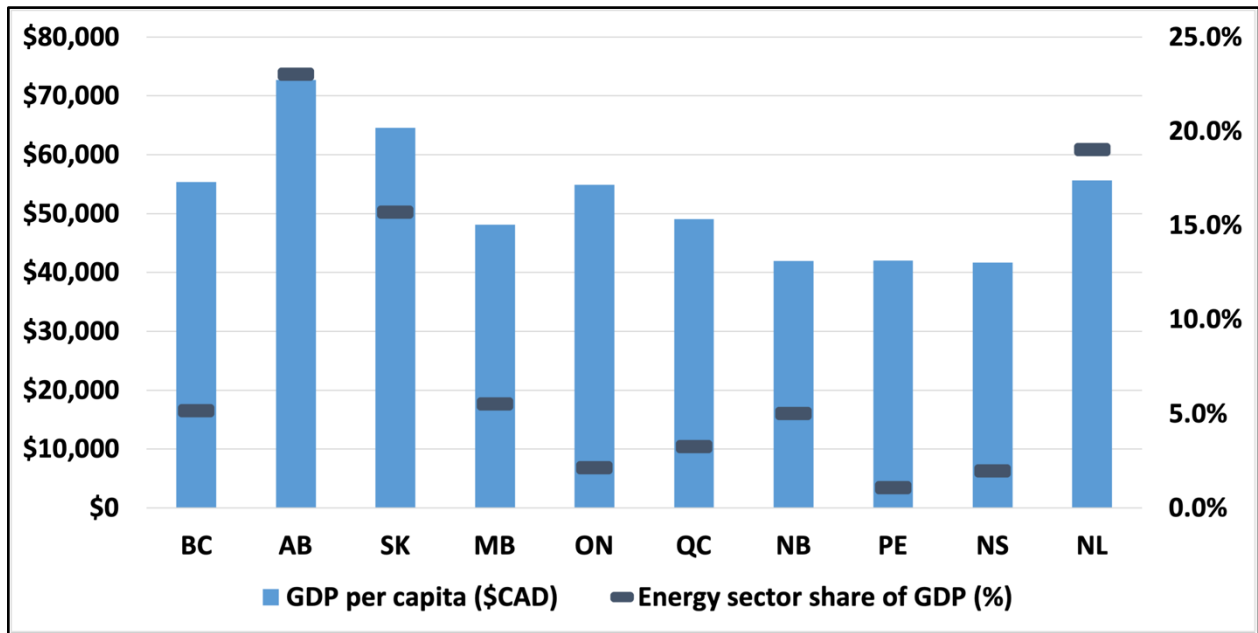


Figure 21 Canadian provincial differences in per capita GDP and energy sector share of GDP [28], [29]

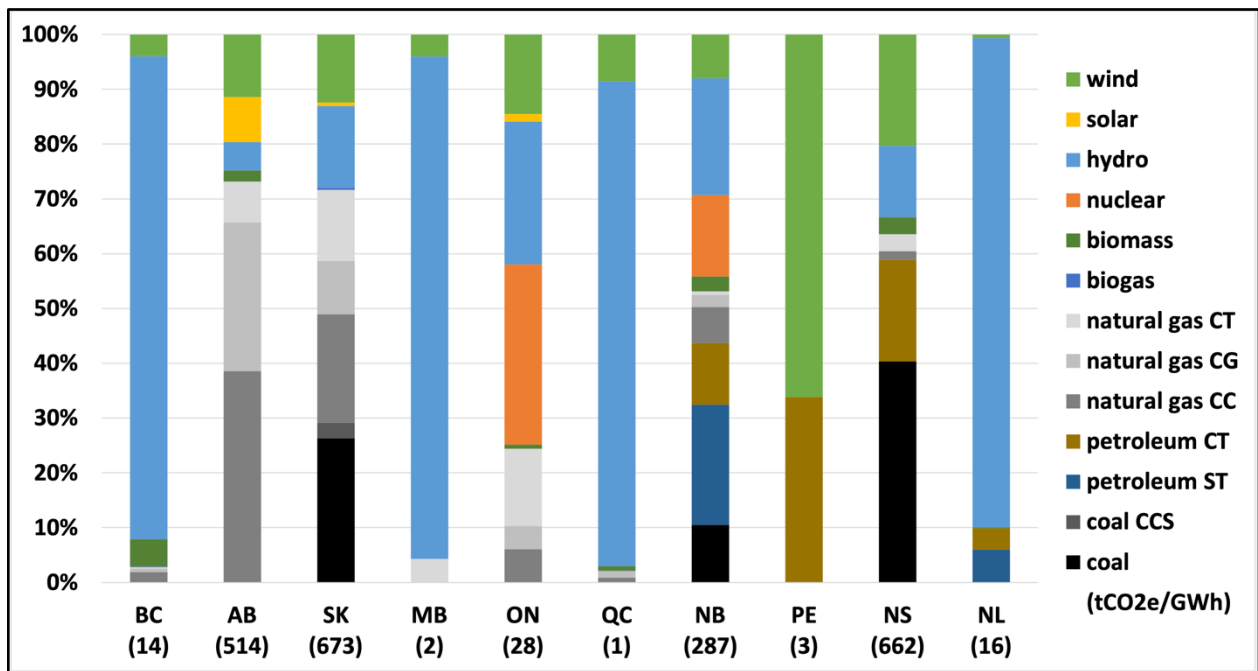


Figure 22 Canadian electricity generation mix and emissions intensities by province

5.3 Methodology

5.3.1 Model development

An ML surrogate methodology is applied to COPPER, a capacity expansion mixed-integer linear planning model, to achieve a more efficient and comprehensive analysis of output variabilities. COPPER determines the least-cost mix of generation and transmission capacity for a specific time period while adhering to power system and policy constraints. The objective function minimizes total system costs including investment, maintenance, production, and carbon costs over the study period (Equation 1).

$$\text{Min } total_system_costs = \min (InvestmentCost + MaintenanceCost + ProductionCost + CarbonCost) \quad (1)$$

COPPER encompasses various optimization constraints, including those related to power balance, planning reserves, thermal generation, hydroelectric development, renewable generation, transmission expansion, and energy storage. Inputs include forecasted electricity demand, existing and future transmission, existing and future generation, and federal and provincial environmental and decarbonization policies. Though valuable for evaluating the effects of carbon pricing and decarbonization policies on grid evolution, COPPER is computationally intensive, which limits its practicality for evaluating outputs under future uncertainties [137].

The current study investigates key Canadian provincial electricity system decarbonization outcomes for 2050. It encompasses carbon emissions, power generation technologies and capacities, and interprovincial transmission capacity. These outcomes offer a comprehensive understanding of power system evolution under select input parameter variations, including carbon prices, demand growth, and generation technology costs (Table 11). Ranges for input variables are based on existing legislation, consultations with subject matter experts, and extension of upper and lower bounds by ~25%, as is common practice in sensitivity analysis [137]. For example, existing carbon pricing legislation increases prices by \$15/t/year from \$65/t in 2023 to \$170/t in 2030 but is unregulated beyond that date [171]. The lower bound envisions prices rising to \$95/t by 2025 (COPPER's base year for carbon pricing) and then remaining unchanged, while the upper bound envisions prices rising to \$95/t by 2025, accelerating by \$30/t/year to \$245/t by 2030, and then incrementally increasing at \$20/t/year to \$645/t in 2050.

Table 10 Selected ranges for input variables

Input variable	Range	Unit	Rationale and References
Carbon tax	95 – 645	\$/t	\$65 in 2023, increasing annually by \$0 to \$30/t to 2030, and thereafter by \$0 to \$20/t to 2050 [137], [172], [171]
Total demand growth 2050/2018	1.2 – 2.5	ratio	Canada's Energy Future Report [173] for 2050, with 2018 as the base year
Annualized capital costs of gas combined cycle	106 – 198	\$/kW	Interquartile range (IQR) determined across these estimates, and used to update the range limits based on the extremes of the identified IQR and the initial limits, as detailed in prior work [172]
Annualized capital costs of gas simple cycle	84 – 145	\$/kW	
Annualized capital costs of diesel	104 – 195	\$/kW	
Annualized capital costs of coal	289 – 549	\$/kW	
Annualized capital costs of nuclear	536 – 972	\$/kW	

Annualized capital costs of biomass	285 – 574	\$/kW	Six literature sources encompassing uncertainties linked to generation technology capital costs, used to transform baseline estimates into equivalent annual payments over a fixed amortization period (CAD\$/kW/year), in line with the original COPPER model formulation.
Annualized capital costs of wind	84 – 242	\$/kW	
Annualized capital costs of solar PV	86 – 216	\$/kW	
Annualized capital costs of battery storage	216 – 463	\$/kW	

5.3.2 Model training

The COPPER model is employed using the input variables in the specified ranges (Table 11). No constraints are imposed on transmission expansion between provinces. This allows a wide array of potential transmission expansion scenarios. Additionally, no target is imposed on emissions reductions, which decline in response to increasing carbon prices and policy constraints. They move towards net-zero but not to zero emissions by 2050. The produced model output data are cleaned to remove outliers and normalized to a common scale. This enables fair comparisons without range distortion or information loss (Equation 2). Outputs having a variance of less than 0.001 are assumed to be constant (model noise). They are ignored in the training process, ensuring a stable and trustworthy base for future analysis and interpretations.

For i in X :

$$\hat{x}_i = \frac{x_i - \min(x_i)}{\max(x_i) - \min(x_i)} \quad (2)$$

The neural network is trained using a dataset of COPPER input and output samples. An empirical model development approach is employed to identify optimal hyperparameters for the model architecture. The selected architecture contains one linear and eight residual blocks, each consisting of two linear layers, two batch normalizations, two dropouts and two ReLu activation functions, with 128 neurons per layer. Batch size, learning rate, and dropout ratio values are 128, 0.001, and 0.5, respectively [137].

The average R-squared value across the entire test dataset is reported in Table 12, alongside training and test errors, and indicates a high goodness of fit of model predictions to test data. This approach ensures a comprehensive assessment of the model's overall performance.

Table 11 Training and Test MSE losses of the model and its accuracy in predictions

Training loss	Test loss	Mean (R2)	Std (R2)
0.0078	0.08	0.94	0.03

In Table 13, the model's run-time and resource use are compared against COPPER. This demonstrates a substantial decrease in computational cost and resource requirements. This efficiency enables more feasible scenario exploration by allowing for as many runs as needed.

Table 12 Comparison of COPPER and surrogate model computational costs and run-time

Model	CPU	Memory	Run-time
COPPER	16 - 32	64 - 128 GB	15h - 72h
Residual neural network	1	NA (Except for saving the model)	12 milliseconds

5.3.3 Output representation

Once the ML model is trained, a sensitivity analysis reveals patterns of evolution in each provincial electricity system to 2050. All inputs are varied within the selected ranges (Table 11) using Latin Hyperbolic Sampling, resulting in over 2000 scenarios. The surrogate model outputs consist of deployments or retirements of generation (in MW) within each province, or expansions in interprovincial transmission transfer capacity (in MW). System parameter impacts on future generation and transmission are shown in histograms for each technology and province. Maximum absolute derivative plots also show standardized outputs against normalized inputs. Computationally demanding, these derivative plots present normalized values demonstrating the relative impact of each input variable on the respective output value. Negative values indicate a negative correlation, positive values a positive correlation, while absolute value represents the strength of correlation. By identifying patterns, this approach provides insights into the relationships between input sensitivities and evolution of each provincial power system to 2050. These graphical approaches are further elaborated in the results presentation.

5.3.4 Model limitations

In conducting this study, several assumptions and limitations were considered. As a mixed-integer linear program optimization model, COPPER has several limitations relevant to interpreting the results of this analysis [12]. This methodology sets specified input ranges, but biases may persist. Rapid changes in decarbonization, demand growth, costs, and technology evolution drive this risk. To reduce computational burdens, COPPER also makes simplifying assumptions including treating transmission and most generation technologies as continuous rather than binary integer variables. A more realistic characterization of generation and transmission development entails modeling contemplated projects with known capacities. A regional analysis of select provinces could reduce computational burdens. COPPER ignores landscape limits that may restrict wind and solar development, possibly overstating potential in some regions. COPPER has few balancing areas and often excludes intraprovincial transmission expansion. This can affect identifying optimized decarbonization pathways. Finally, imports and exports are modeled using historical data due to future uncertainty. Major trade changes could affect optimal decarbonization pathways. Future modelling could consider varying electricity trade patterns to provide policy insights into domestic decarbonization pathways.

Despite its advantages, the surrogate ML model approach also has limitations in addition to those associated with COPPER. For dataset generation, COPPER's default constraints were applied to represent practical and non-contentious pathways. One key limitation is the potential loss of granularity and accuracy due to simplified

representations that do not fully capture nuances in the COPPER formulation. Secondly, the reliability of the surrogate model depends upon the quality and comprehensiveness of the training data, so extrapolating the model's predictions beyond the training data could lead to unreliable results. The ML model shows less sensitivity to parameters with small normalized values. This may lower predictive accuracy for small-valued outputs in some provinces, though they are not the focus here. Furthermore, as COPPER evolves and incorporates new features, this ML surrogate model will require retraining to maintain accuracy. Lastly, while the surrogate model provides predictive power, understanding the specific reasons behind its predictions can be challenging, which may impact its overall interpretability.

5.4 Results

The results of this work are presented as national and provincial summaries in terms of additions of renewable generation (wind and solar), additions and retirements of natural gas generation, and expansions of inter-provincial transmission. Results are mostly non-constant, varying with input sensitivities. Such variations are often more relevant to policymakers [137], [172]. Coal generation results are omitted. This technology retires rapidly in all provinces due to high emissions, fuel costs, and rising carbon prices. Selection of results focuses on key provincial pairings including British Columbia (BC) – Alberta (AB), Saskatchewan (SK) – Manitoba (MB), and Ontario (ON) – Quebec (QC). These regions hold over 90% of Canada's generation capacity. Transmission expansion is under review for grid decarbonization.

5.4.1 Renewable generation

Table 14 summarizes results for modeled wind and solar development within each Canadian province. Existing installed capacities reflect current installations of utility-scale wind and solar generation and exclude planned additions. Wind generation currently operates in all provinces, while most provinces do not currently have installed utility-scale solar generation. Scenarios with no additional capacity reflect the proportion of modeled scenarios in which no wind or solar is developed to 2050. Mean and maximum additional installed capacity provide insights into the magnitude of the potential buildout of these technologies to 2050 within each province.

Table 13 Modeled wind and solar development by Province

Province	WIND					SOLAR				
	Existing	Additions				Existing	Additions			
	Installed capacity	Scenarios with no additional capacity	Mean additional installed capacity	Mean additional capacity above existing	Maximum additional installed capacity	Installed capacity	Scenarios with no additional capacity	Mean additional installed capacity	Mean additional capacity above existing	Maximum additional installed capacity
	(GW)	(%)	(GW)	(%)	(GW)	(GW)	(%)	(GW)	(%)	(GW)
BC	0.7	54%	4.3	582%	49.4	0.0	11%	25.2	n/a	72.2
AB	4.8	2%	27.3	567%	62.7	2.3	72%	2.9	126%	66.0
SK	0.6	0%	3.6	569%	8.9	0.0	78%	0.3	1093%	16.4
MB	0.3	2%	1.5	600%	3.5	0.0	91%	0.1	n/a	8.2
ON	4.9	1%	6.8	140%	19.3	0.5	41%	2.7	564%	26.5
QC	3.9	34%	0.5	13%	4.1	0.0	42%	3.2	n/a	21.0
NB	0.4	100%	0.0	0%	0.0	0.0	26%	0.7	n/a	3.7
PE	0.2	2%	0.6	285%	2.1	0.0	74%	0.1	n/a	1.4
NS	0.6	23%	0.4	66%	2.7	0.0	4%	1.1	n/a	2.6
NL	0.1	4%	0.7	1315%	1.3	0.0	24%	0.8	n/a	3.9
TOTAL	16.5		45.8		154.0	2.8		37.1		221.8

Findings indicate that six provinces (AB, MB, ON, PE, NL, SK) develop wind robustly. Few scenarios show no added capacity by 2050. In three provinces (BC, QC and NS) the extent of wind development depends strongly on inputs. Only one province (NB) lacks additional wind development due to anticipated low demand growth [174]. Solar development occurs in all provinces but varies substantially by proportion of scenarios with no utility-scale solar development (4% to 91%), by mean (0.1 to 25.2 GW) and by maximum (1.4 to 72.2 GW) developed capacity. Provinces developing significant wind (solar) resources are less likely to also develop significant solar (wind) resources.

British Columbia and Alberta. In BC, wind energy development exhibits high robustness, displaying limited sensitivity to input variations, as more than half of the ~2000 scenarios develop no new wind (Figure 23). The y-axis on this histogram presents the count of scenarios returning technology deployment values within each bin across the maximum range of values. The x-axis contains normalized values in standard deviations from the mean, with negative values indicating scenarios where values fall below the average. Specifically, mean wind deployment in BC to 2050 totals ~4.3 GW (4,344 MW), ranging between 0 GW in ~1100 scenarios up to ~49.4 GW (6 s.d.) in the most extreme scenario. This insensitivity to inputs implies a relatively stable path of limited future wind energy development in BC, a finding further explored in the Discussion.

Contrastingly, solar development in BC shows higher variability and uncertainty. It is influenced by policies, carbon tax, capital costs, and electricity demand in BC and Alberta (Figure 23). The derivatives plot illustrates the effect of each of six factors on solar generation in BC to 2050. The maximum absolute derivative value indicates the steepest slope or the maximum change of one variable in relation to the other. Higher carbon taxes, higher wind costs, and lower solar costs increase solar development. Demand and natural gas capital costs have a smaller impact.

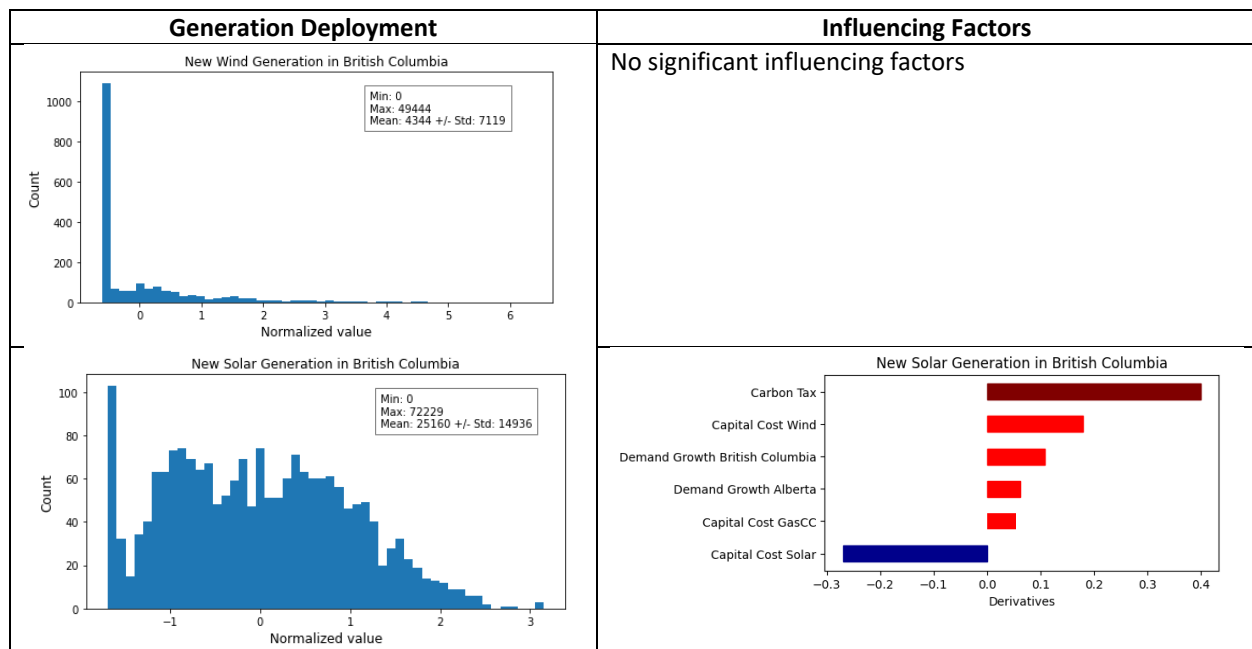


Figure 23 Wind and Solar Generation in BC – Deployment and Influencing Factors

Wind energy is likely to play a substantial role in Alberta’s energy future regardless of evolving circumstances. Substantial new wind (mean ~27 GW) is developed to 2050, with larger capacity buildouts under a significant minority of scenarios (Figure 24). The carbon tax is the primary factor influencing wind development, followed by lower wind capital costs and higher solar capital costs. Despite variations in inputs, solar development in Alberta reflects lower sensitivity to input changes (and lower overall development) compared to wind energy (Figure 24).

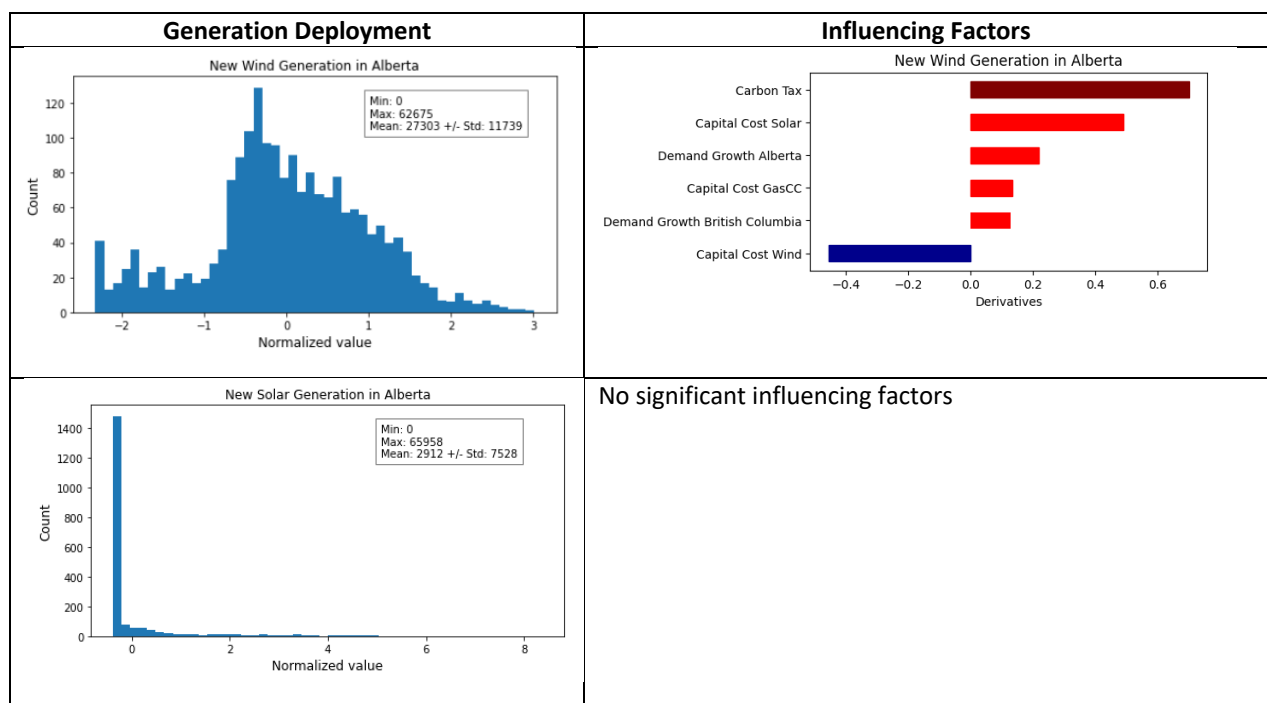


Figure 24 Wind Generation in Alberta - Deployment and Factors

Saskatchewan and Manitoba. There are wide variations in the quantities of wind developed in Saskatchewan and Manitoba (Figure 25). In almost all scenarios (> 95%), new wind generation capacity is developed in Saskatchewan (>1000 MW) and in Manitoba (> 500 MW) by 2050. In rare scenarios consisting of low carbon prices, low demand and high technology costs is no wind developed in either province. No new solar development occurs in most scenarios in Saskatchewan (>75%) and in Manitoba (>90%) suggesting a robust pathway of limited development to 2050 (Table 14). Mean solar development is relatively low in Saskatchewan (~300 MW) and lower still in Manitoba (~150 MW), while additional development occurs where future solar capital costs decline compared to wind capital costs (Figure 25).

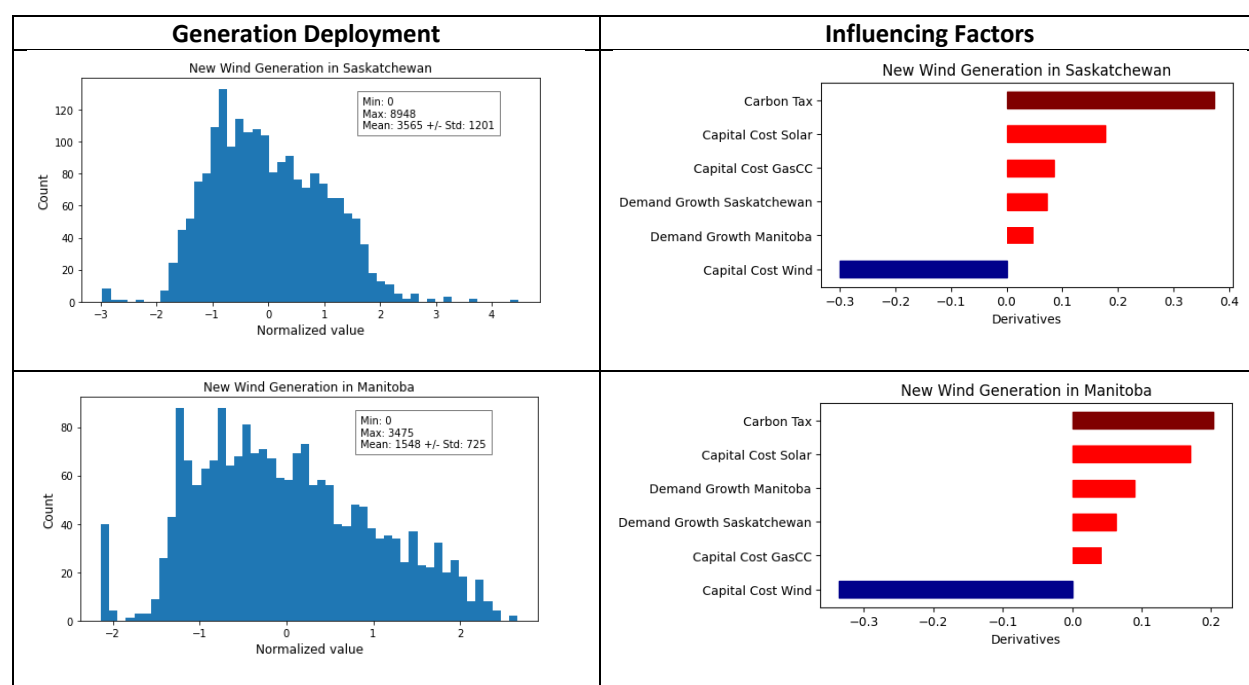


Figure 25 Wind Generation in Saskatchewan and Manitoba - Deployment and Factors

Ontario and Quebec. Wind energy will grow in Ontario's electricity system. Carbon prices and cost differences between wind and solar will drive this growth. Mean additional development by 2050 is substantial (~7 GW), and only in rare scenarios of high wind costs, low solar costs, low demand, and low carbon prices is no new wind energy developed in Ontario (Figure 26). In a majority of scenarios (~60%), new solar generation is developed in Ontario with mean development (~2.7 GW) indicating a somewhat less robust path compared to wind development.

In nearly two-thirds of scenarios, additional wind is developed in Quebec, though compared to existing installed capacity (~4 GW) mean development (~0.5 GW) is modest. As in Ontario, in a majority of scenarios (~60%) new solar generation is developed in Quebec, though unlike in Ontario mean solar development (3.2 GW) exceeds mean wind development. The lack of development scenarios including either wind (34%) or solar (42%) in Quebec illustrates significant dependencies of wind and solar build-out on input conditions. Future wind deployment in Quebec is driven by carbon prices and wind-solar cost differences. Demand in Quebec and nearby provinces has a smaller effect while no single factor drives solar deployment in Quebec or Ontario.

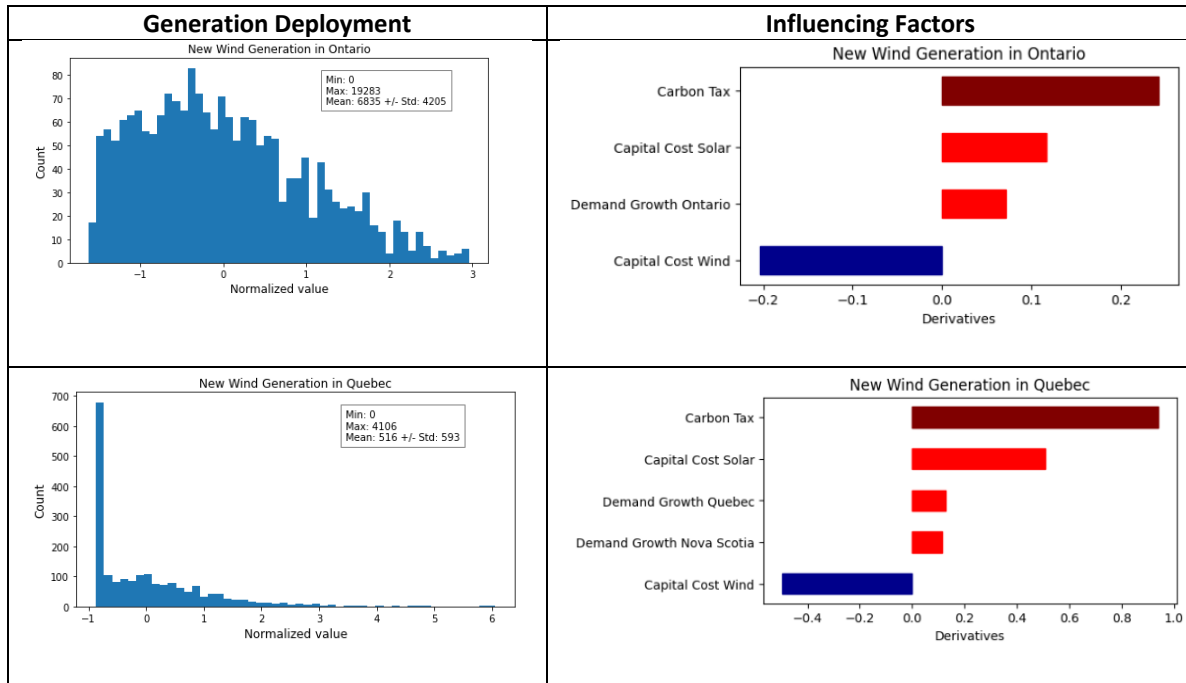


Figure 26 Wind and Solar Generation in Ontario and Quebec – Deployment and Factors

5.4.2 Natural gas generation

Findings for natural gas generation indicate pathways to deep decarbonization in all provinces do not retire these generating assets almost regardless of input variables (Table 15). This result is facilitated by the model's lack of a hard constraint on emissions, which decline to net-zero but not to zero by 2050. Natural gas additions are limited to combined cycle generation, which has lower modeled capital and operating costs compared to simple cycle generation. For all provinces, with the exception of BC, natural gas additions are minimal with substantial additions occurring only under very extreme circumstances. This flexible thermal generation and hydroelectric generation, supports integration of increasing quantities of variable renewable generation. They also provide contingency and reserve capacity. This indicates a robust pathway for existing installed natural gas generation to support decarbonization into the foreseeable future.

Table 14 Modeled natural gas development by Province

NATURAL GAS COMBINED CYCLE							
	Existing	Retirements			Additions		
Province	Installed capacity	Scenarios with no capacity retirement	Mean capacity retired	Maximum capacity retired	Scenarios with no capacity additions	Mean additional installed capacity	Maximum additional installed capacity
	(GW)	(%)	(GW)	(GW)	(%)	(GW)	(GW)
BC	0.2	100%	0.0	0.0	18%	4.3	15.6
AB	13.5	55%	1.3	9.4	90%	0.3	10.7
SK	1.5	84%	0.0	1.1	95%	0.0	2.3
MB	0.0	100%	0.0	0.0	95%	0.0	1.3
ON	3.5	78%	0.1	0.5	89%	0.1	5.9
QC	1.0	55%	0.3	1.0	100%	0.0	0.0
NB	0.4	98%	0.0	0.1	91%	0.0	1.1
PE							
NS	0.0	87%	0.0	0.3	81%	0.0	0.4
NL							
NATURAL GAS SIMPLE CYCLE							
	Existing	Retirements			Additions		
Province	Installed capacity	Scenarios with no capacity retirement	Mean capacity retired	Maximum capacity retired	Scenarios with no capacity additions	Mean additional installed capacity	Maximum additional installed capacity
	(GW)	(%)	(GW)	(GW)	(%)	(GW)	(GW)
BC	0.0	95%	0.0	0.0	100%	0.0	0.0
AB	1.3	95%	0.0	1.1	100%	0.0	0.0
SK	0.6	95%	0.0	0.7	100%	0.0	0.0
MB	0.3	95%	0.0	0.4	100%	0.0	0.0
ON	6.9	100%	0.0	0.0	100%	0.0	0.0
QC	0.0	100%	0.0	0.0	100%	0.0	0.0
NB	0.0	100%	0.0	0.0	100%	0.0	0.0
PE							
NS	0.1	100%	0.0	0.0	100%	0.0	0.0
NL							

Note: Gray cells indicate the generation type does not exist in this province.

In BC, in contrast to other provinces, there is significant (mean 4.3 GW) expansion in new natural gas combined cycle generation. This consistent selection of new natural gas generation reflects its lower costs compared to other forms of dependable and flexible capacity. This includes hydroelectric generation and energy storage, and that nuclear

generation is prohibited in BC [163]. Existing combined cycle generation under all scenarios and simple cycle under most scenarios (95%) remains operational until 2050 (Figure 27).

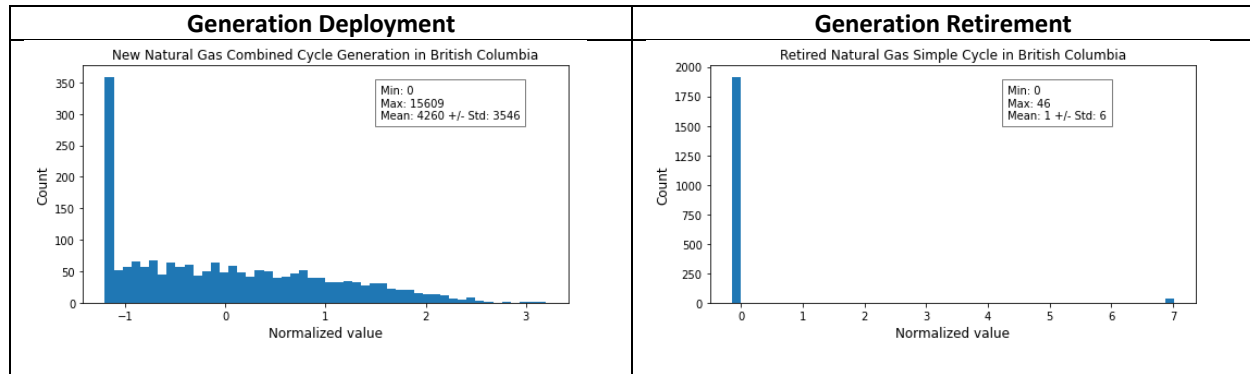


Figure 27 Natural Gas Generation in BC – Deployment and Retirement

5.4.3 Interprovincial transmission

For all three provincial pairings investigated, a majority of scenarios see additional transmission transfer capacity between jurisdictions. This suggests an important role for transmission expansion in grid decarbonization in Canada (Table 16).

Table 15 Modeled transmission transfer additions by provincial pairs

TRANSMISSION						
Province	Province	Existing		Additions		
		--> transfer capacity	<-- transfer capacity	Scenarios with no additional capacity	Mean additional transfer capacity	Maximum additional transfer capacity
		(GW)	(GW)	(%)	(GW)	(GW)
BC	AB	1.00	0.80	42%	1.50	9.00
SK	MB	0.15	0.40	17%	0.22	1.03
ON	QC	2.04	2.67	27%	1.05	4.95

Note: While existing transfer capacities are presented unidirectionally, the modeled transmission additions are bi-directional.

In the majority of scenarios, additional transmission transfer capacity is developed between BC-Alberta (~60%), Saskatchewan-Manitoba (~85%), and Ontario-Quebec (~75%), with modeled development varying under different input conditions. Influencing factors across provincial pairings include higher wind costs reducing transmission development, and higher carbon taxes, higher solar costs and, to a lesser degree, demand growth increasing development. A high carbon tax results in more rapid decarbonization in provinces with comparatively higher emissions intensities (AB, SK, ON). This triggers more interconnection with highly decarbonized neighbouring provinces (BC, MB, QC). Lower wind generation capital costs increase wind capacity. This results in larger surplus generation best utilized in neighbouring jurisdictions by developing additional interprovincial transmission. As solar

capital costs decrease, the installed transmission between provinces decreases, an intriguing result explored further in the Discussion.

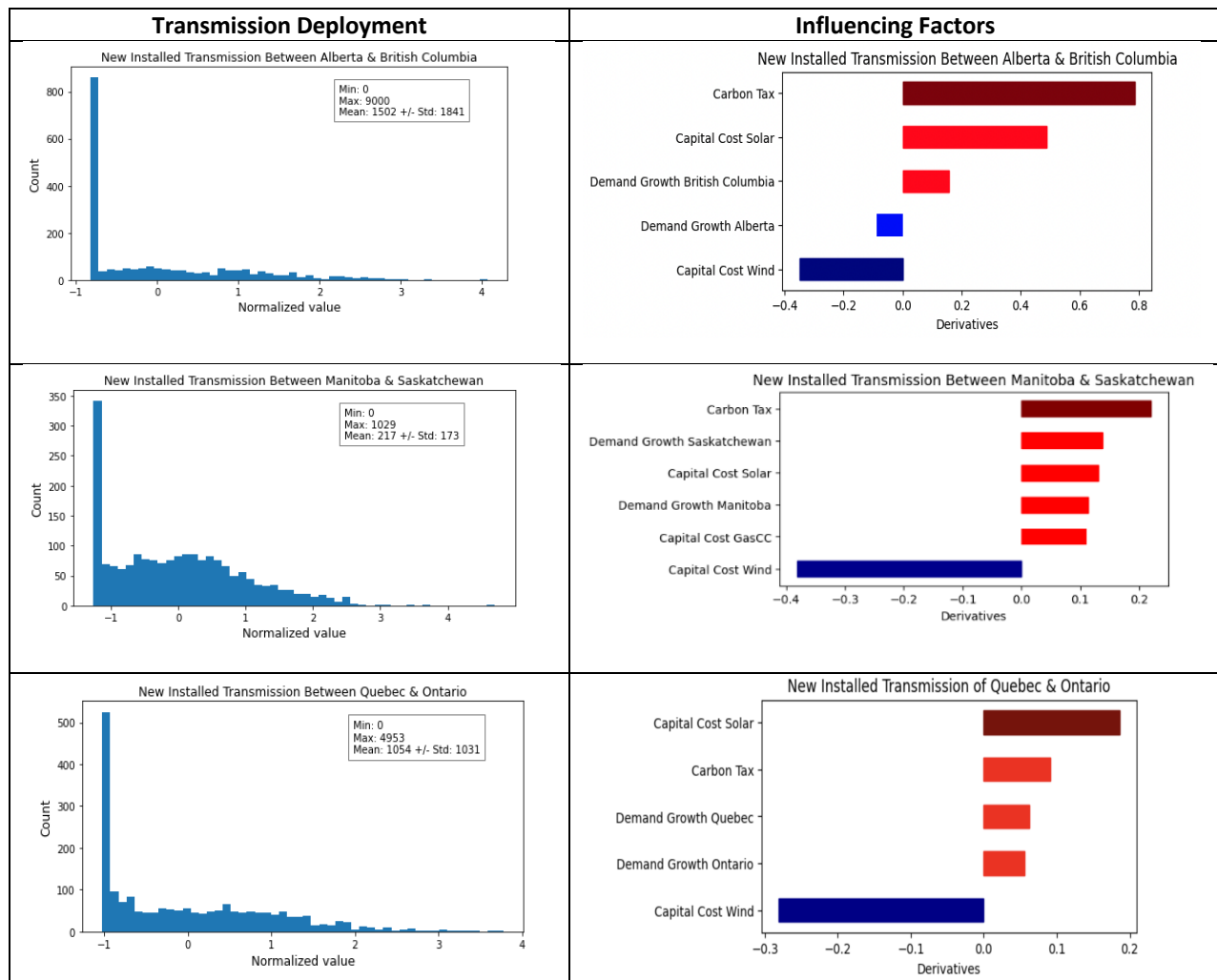


Figure 28 Transmission between provinces – Deployment and Factors

5.5 Discussion

This investigation aims to give policymakers insights into least-cost, robust pathways to net-zero in Canadian provincial electricity systems. Specific policy implications discussed below include those related to the federal *Greenhouse Gas Pollution Pricing Act*, *Clean Investment Tax Credit* and *Clean Electricity Regulations*, the recently announced Alberta renewables policy and the *BC Clean Electricity Delivery Standard*. A secondary interest is to investigate the potential of ML models to analyze least-cost optimization of power systems to net-zero emissions in response to uncertainties and variability in technology capital costs, electricity demand, and carbon pricing.

5.5.1 Renewable Generation

Our findings indicate that four provinces need to plan for significant new wind development to 2050. This includes Alberta (mean 27.3 GW, max. 62.7 GW), Ontario (mean 6.8 GW, max. 19.3 GW), Saskatchewan (mean 3.6 GW, max

8.9 GW) and Manitoba (mean 1.5 GW, max 3.5 GW), with other provinces also likely to see additional wind development (Table 11). Solar development occurs in all provinces but varies substantially in terms of developed capacity. The main driver of deployment is the federal carbon tax. Raising carbon prices beyond 2030, as mandated by the Greenhouse Gas Pollution Pricing Act, is crucial for deep decarbonization. Technology capital costs also play a prominent role in driving renewables deployment. The recently proposed *Federal Clean Electricity Investment Tax Credit* introduces a 15% refundable tax credit for non-emitting electricity generation, including wind, solar and abated natural gas generation, as well as interprovincial transmission [175]. The investment tax credit must stay predictable yet adaptable. It should respond to cost stagnation and rapid declines, as seen in wind and solar trend [176], [177].

At the provincial level, Alberta has high suitability for both wind and solar generation, most (72%) of the investigated scenarios suggest no additional solar capacity to 2050, and modest mean future solar development (~3 GW) compared to wind (~27 GW) (Figure 24). This can be explained by the differing contribution of wind and solar generation to reserve requirements. Meeting these reserves is harder in Alberta's decarbonized grid due to limited hydro supply (Figure 22). The estimated year-round effective load carrying capability (ELCC) of wind generation (16%) in Alberta [178] makes a meaningful dependable capacity. This reduces the need for natural gas capacity. The estimated ELCC of solar generation in Alberta in summer (20%) and winter (0%) means that solar makes no winter contribution to reserve requirements in Alberta, a winter-peaking system [178], [179]. This reserve contribution difference tilts the preference toward wind over solar generation in Alberta. Nationally, the ELCC of wind generation is typically 15% to 35% of installed capacity with higher contributions in winter than summer [180], [178], [181]. Across Canadian provinces, solar generation makes no contribution to winter reserve requirements, though almost all provincial systems are winter peaking [180], [178], [181]. Wind generation thus has a larger impact compared to solar generation in reducing the need for higher-emitting load-balancing generation. Cost is not the sole factor determining whether to proceed with wind or solar generation as operational considerations are also relevant [182].

Alberta recently placed a seven-month pause on utility board approvals related to wind and solar facilities to conduct an inquiry into environmental impacts, site reclamation, and electricity system reliability [32]. In response to inquiry findings, the Government of Alberta announced a prohibition on wind and solar development on Class 1 and 2 agricultural lands. Wind projects are also banned within 35 km of protected areas [183]. This recent policy direction would preclude wind, and to a lesser extent solar, development over large areas of Alberta not considered in the current analysis. Further investigation should assess this new policy's impact. It may restrict lower-cost sites for wind and solar development. As a result, a higher carbon price would be required to shift deployment towards renewables and away from natural gas, delaying decarbonization. The sum of modeled mean wind deployment across all provinces in the current analysis (~46 GW) vastly exceeds total existing installed capacity (~16 GW) (Table 14). This deployment needs policy alignment across all government levels. Collaboration should consider rural, agricultural, health, species protection, and wilderness values [184]. Neither COPPER nor the current ML model account for these landscape variables that could preclude wind development. Future modeling could utilize the current ML model to

test variations in land availability (e.g., parklands, agricultural lands, waterbodies, etc.) and consequent effects on generation technology deployment and system costs.

In BC, solar generation may be poised for significant expansion under appropriate cost and policy conditions. Modeled mean solar development (~25 GW) far exceeds wind (~4 GW). This occurs despite wind being Alberta's lowest-cost low-carbon energy source [180]. Two factors potentially contribute to this result. First, requirements for additional generation in BC are delayed due to the Site C Project, a large (1,100 MW, 5,200 GWh/y) hydroelectric facility that enters the COPPER model in 2025. Since our modelling inputs include greater declines over time in the capital costs of solar generation compared to wind generation, this delay results in greater proportional solar deployment into the future. Additionally, prime solar development locations in BC are relatively proximal to the existing transmission network. These results in comparatively lower transmission interconnection costs.

5.5.2 Fossil Generation

Provincial electricity system operators plan for significant emissions reductions by taking different approaches to retirements, operations, and renewals of existing fossil-fueled generation. The Ontario Independent Electricity System Operator found natural gas provides dependable capacity, quick response, ramping, reliability, and reserve support [39]. These traits are hard to replace. Low-carbon alternatives are costly and need long lead times. Storage and demand response would be required in unattainable amounts, keeping natural gas in use beyond 2035 [39], [185]. Furthermore, a rapid phase-out of natural gas generation in Ontario would result in frequent blackouts [185]. Similarly, the Alberta Electricity System Operator found net-zero pathways by 2035 uncertain and costly. They required verified offsets and widespread use of unproven technologies [40]. For its part, Hydro Québec plans to retain and convert natural gas generation to non-emitting fuels. This ensures continued operational benefits and reserve support [186].

Contrastingly, BC Hydro is implementing a 100% Clean Electricity Delivery Standard. It plans to phase out of remaining natural gas generation by 2030 [38], which may conflict with the current study's findings. While most modeled scenarios across all provinces (>90%) see no new natural gas development (Table 15), the current analysis indicates that least-cost decarbonization pathways develop significant natural gas generation (mean ~4.3 GW) in BC to 2050. This finding aligns with a recent continental decarbonization study. It showed continued natural gas development in BC and Alberta through 2050 [24], [36]. A recent study on 100% clean electricity in the US by 2035 found natural gas turbines provide 21% of dependable capacity but only 4% of annual energy [37]. Emissions from unabated generation can be offset, but decarbonizing the last portion of electricity emissions is costly [37]. Advancing BC's 100% Clean Electricity Delivery Standard, phasing out natural gas by 2030 and banning new unabated generation [38], should involve careful review of alternatives. Options include retaining natural gas, exploring low-carbon fuels [173] and carbon offsets [40], to manage grid decarbonization costs.

The current analysis models to the policy context in place at the time of modelling, while policy is rapidly evolving in response to decarbonization imperatives. In August 2023, the Canadian government introduced Draft Clean

Electricity Regulations (CER). They set a revised emissions limit of 30 tCO₂e/GWh for interconnected fossil-fueled generation, effective January 1, 2035, or 20 years after commissioning, whichever is later [41]. More recently, Environment Canada proposed raising the emissions standard. This change would allow abated natural gas generation with carbon capture and storage, mainly for load-following or peaking use, which cannot meet the stricter limit [41]. Consistent with these proposed revisions, the analysis shows robust decarbonization pathways. Most natural gas generation stays online but operates less often as the system decarbonizes. In this analysis, the carbon tax is the most influential factor affecting generation and transmission development and acts as the primary constraint on the retirement and deployment of natural gas generation. In terms of retirements, after 2035, the lower performance standard in the Draft CER would reduce annual capacity factors at many facilities. This could lead to earlier retirements than forecasted in the current analysis. The low capital cost of natural gas units may lead the Draft CER to trigger retrofits to non-emitting fuels. This would help meet emissions targets while ensuring reliability. The analysis projects no significant gas deployments except in BC, so the Draft CER would not greatly change these results.

5.5.3 Transmission

Results for interprovincial transmission development provide insights into the complex interactions between carbon taxes, generation technology costs and electricity demand. Findings for the three provincial pairings investigated indicate that lower wind generation capital costs increase transmission development between provinces. While lower solar generation costs decrease development. Lower wind capital costs lead to more wind deployment and larger surplus generation. This surplus, both daily and seasonal, is managed through exports via expanded interprovincial transmission. Transmission expansion uses geographic wind variability across provinces. It enables exports during surpluses and imports during shortfalls. Contrastingly, lower solar capital costs increase solar deployment and create larger intra-daily surpluses. These surpluses are managed more cost-effectively by shifting load-following generation than expanding interprovincial transmission.

Increasing electricity demand also influences transmission development, though to a lesser extent than carbon taxes and wind capital costs. In general, demand in the province in which less wind development is projected has a greater influence on interprovincial transmission development. In other words, increasing demand in BC, MB, and QC influences interprovincial transmission development more than does increasing demand in AB, SK or ON. This result is unsurprising considering that wind generation creates surpluses best used by neighboring provinces. However, interprovincial transmission development depends on sufficient demand.

In the case of Ontario-Quebec transmission, solar capital costs influence the need for new transmission more than do higher carbon taxes, a unique result. Higher solar capital costs also increase wind development in Quebec (Figure 28). As solar capital costs rise, investing in additional transmission becomes preferable. This allows greater electricity trade between the provinces. In the case of BC-Alberta, the factor analysis suggests a similar mechanism driving transmission development as between Ontario and Quebec (Figure 28). The additional findings that wind

development is preferred in Alberta and solar development in BC suggest that given lower wind capital costs, Alberta develops large quantities of wind along with transmission to support exports to BC. This is supported by the additional influence of demand growth in BC on transmission development between the provinces (Figure 28). However, with lower solar capital costs, each province develops its own resources. BC focuses on solar, Alberta on wind, without expanding interprovincial transmission.

The complex links between solar costs, wind costs, and transmission affect policymaking. They impact funding decisions under the *Clean Investment Tax Credit*. Specifically, a future drop in solar costs compared to wind suggests less need for interprovincial transmission investment. It points to increased investment in technologies like energy storage and abated natural gas for balancing solar variations. Contrastingly, a marked decline in the costs of electricity from wind relative to solar generation indicates a need for greater investment in interprovincial transmission. Incentives and investments in interprovincial transmission should be strategically considered in terms of the evolution of wind and solar generation technology costs.

5.6 Conclusions

This research investigates the potential of ML models to analyze least-cost decarbonization of provincial power systems across Canada in response to uncertainties and variability in technology capital costs, electricity demand growth, and carbon pricing. The study provides several insights into robust pathways respecting wind and solar generation, reducing emissions from natural gas generation, and expanding Canadian interprovincial transmission that remain robust under many uncertainties and variabilities.

Findings indicate robust conditions for substantially expanded wind generation but less robust conditions for expanded solar generation in the decarbonization of Canada's provincial electricity grids. Most provinces develop wind under almost all future scenarios, with the potential exception of British Columbia, where higher-cost wind generation results in solar generation becoming the primary low-carbon electrical energy source.

Canadian policy increasingly focuses on grid decarbonization. However, the analysis shows natural gas generation remains but operates infrequently in most scenarios. This supports policies maintaining gas for reliability and reserves. Almost no new natural gas is developed under any scenarios, with the noted exception of British Columbia. Carbon prices, along with wind and solar capital costs, act as primary determinants of least-cost decarbonization pathways. Planners and policymakers should optimize existing natural gas use while planning a gradual emissions phase-out. This approach balances decarbonization goals with system reliability.

In terms of interprovincial transmission, our findings indicate that provinces should proactively and strategically explore opportunities to enhance transmission transfer capabilities. This ensures efficient energy exchange to meet regional demands. This exploration, including potential federal investment, should consider how lower wind costs can drive interprovincial transmission development in least-cost decarbonization pathways. Lower solar costs, however, reduce the need for such transmission.

Recent analyses of deep decarbonization pathways show significant future wind and solar development across Canada [12], [39], [40]. The extent of development in each province depends on factors like demand growth, technology costs, and decarbonization policies, including carbon prices. However, other potential factors not considered here include variations in the quality of the wind resource (i.e., wind speed) or solar resource (i.e., insolation), the distance from these resources to load centers, the influence of landscape characteristics, and the costs of interprovincial transmission. Resource quality and distance to grid are inputs to COPPER and considered to be accurately quantified with limited potential for variation. Future modeling could further test the influence of variations in land availability and interprovincial transmission capital costs on grid decarbonization in Canadian provinces.

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Data Availability

Our code for generating data, developing the model, and visualizing the results is available at https://github.com/ZahraJahangiri/DL_COPPER.

The raw data for training the ML model is available on the SESIT website (<https://sesit.cive.uvic.ca/>) Under Zahra Jahangiri's profile, with a direct link at <https://sesit.dev/zahra/download>.

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Author Contributions

Z. J. contributed to conceptualization, methodology, software, validation, formal analysis, investigation, writing (original draft), and visualization, R.H. contributed to conceptualization, and writing (original draft) and visualization, M. M. contributed to supervision, resources, writing (reviewing and editing), and funding acquisition.

6 Conclusion, policy implications, and future work

6.1 Conclusion

Power system planning requires better strategies and tools. Energy systems have underutilized ML in planning and decarbonization. Computational models with long run times and high demands hinder efficiency. They also add to global warming through operational resource use. This thesis highlights ML's potential in improving power system planning by exploring the design space. It presents a novel approach to modeling and decision-making. The goal is to support informed planning for decarbonization.

Chapter Two presents a survey on ML techniques and their applications. It focuses on their role in power systems and policy. The chapter examines ML methods and their use in operations. It also discusses their impact on policy and regulations.

In Chapter Three, a surrogate model was developed using deep neural networks to reduce computational time and resource demands. The model enables efficient exploration of the electricity sector's design space. It supports scenario exploration, sensitivity analysis, and uncertainty analysis. Run time was reduced from 11–72 hours to 17 milliseconds. Computational requirements decreased from 16–32 CPUs and 64–128 GB of memory to 1 CPU and 50 MB of memory. This work uncovers relationships between policy inputs and system outcomes. It addresses gaps in the use of ML for large-scale energy systems. The goal is to extract insights for planning toward decarbonization. The COPPER model, known for modeling high-resolution spatiotemporal constraints and policy options, was employed. Despite its capabilities, the COPPER model is computationally demanding. This work overcomes those challenges to efficiently explore the design space, particularly for sensitivity and uncertainty analysis. A visualization method using K-means clustering, heat maps, and ranked bar charts simplifies insight communication. This approach extends the surrogate modeling methodology, offering tools to address diverse research questions.

Chapter Four introduces a new perspective to power system modeling. It emphasizes the need to address uncertainties in modeling and policy planning. The main goal is to provide insights into system behavior, causative factors, and decarbonization pathways. This work addresses limitations in current modeling approaches. It highlights areas for further research and offers guidance for policymakers. The study integrates ML and numerical analysis to refine modeling approaches. It stresses the importance of incorporating uncertainties in input parameters. Another contribution of this chapter is the research and exploration conducted to identify proper input parameter. This ensures a reliable and comprehensive estimation of real-life scenarios. Using the new dataset, a more accurate surrogate model was developed and applied for uncertainty analysis. These efforts reveal correlations not immediately apparent and offer insights beyond intuitive assumptions. The findings suggest that applying these methodologies at a provincial level could provide specific insights for policy planning.

In Chapter Five, ML models were used to analyze the least-cost optimization of provincial power systems across Canada. The study focused on achieving net-zero emissions and addressing provincial differences in power systems for effective decarbonization. The analysis included uncertainties in technology costs, electricity demand growth,

and carbon pricing. It examined the evolution of provincial power systems and interprovincial transmission. The goal was to provide insights for planning and policymaking at the provincial level. The study explored least-cost decarbonization pathways that remain robust despite uncertainties. This chapter, highlighted pathways heavily influenced by these variabilities. In this study, the input dataset from previous work, which included the identified proper parameter ranges, was used. However, the output dataset focused on provincial variables, and the model was developed using these provincial-specific variables. Sensitivity and uncertainty analyses were then conducted using the provincial surrogate model to provide detailed insights for each province.

This study highlighted carbon taxes and wind capital costs as key factors. These parameters significantly impact electricity system outcomes. The findings reaffirm Canada's commitment to carbon pricing. The next decade is pivotal for electricity system decarbonization. Regional variations will play a crucial role in this evolution.

This study highlighted the importance of uncertainties in capacity factors on power system outcomes. Gas CC power, with its lower emissions, is less affected by carbon taxes. It supports large wind and solar integration, even at high tax rates. Hydroelectric power, a key part of Canada's energy mix, showed consistent stability. However, its future role may need reassessment due to current concerns. Transmission expansion patterns reflected VRE capacity variability across locations. This underscores the importance of transmission in decarbonization. Nuclear and diesel roles were significantly reduced. Carbon emissions, gas CC, and solar power emerged as critical determinants. Solar showed a more prominent role than wind in future scenarios.

In the broader landscape, wind generation is set for significant growth across Canada's provincial grids. The future of utility-scale solar in decarbonization remains uncertain. In British Columbia, remote wind resources may lead to solar playing a larger role. The net-zero target by 2035 suggests natural gas will mainly serve peak demands. British Columbia's potential to develop new natural gas facilities for deeper decarbonization was noted. Enhancing inter-provincial transmission is critical for efficient energy exchange. Factors influencing transmission development vary significantly across provinces.

These findings provide a detailed view of the Canadian electricity system's dynamics and its transformation, guided by ML and numerical analysis. Central to this research was the surrogate model, which produced extensive input-output correlation plots. With its ability to run in milliseconds and minimal hardware requirements, the model can integrate with real-time tools and systems. This integration enables dynamic decision-making, continuous optimization, and proactive energy management. The model's applications extend to real-time grid balancing, scenario analysis for renewable integration, and adaptive policy planning.

Innovative visualization methods, including interactive dashboards, enhance usability by presenting these insights in an accessible format. These tools allow policymakers, energy planners, and utility operators to explore scenarios, monitor system performance, and make informed decisions efficiently. This comprehensive approach positions the surrogate model as a versatile and indispensable tool for advancing decarbonization efforts in Canada.

The surrogate model analysis provided new insights not available from single-model studies. This thesis introduces tools and perspectives for power system researchers. These tools were developed using current policy and programming knowledge. To stay relevant, they should be updated with recent policies. They can also be enhanced for broader domain-related studies.

6.2 Summary of Contributions

This thesis advances power system planning for deep decarbonization by integrating machine learning with large-scale, policy-aware energy system modeling and by centering the analysis on the full output space that this integration makes tractable. Conventional capacity expansion and decarbonization studies are typically constrained to a small set of scenarios or point estimates, suffer from prohibitive computational costs, and under-treat the structure of uncertainty and interdependencies among outcomes. In contrast, this work develops and operationalizes a methodological ecosystem that (i) dramatically reduces computational barriers via surrogate modeling, (ii) enables systematic exploration of high-dimensional input and output spaces, (iii) incorporates rigorous uncertainty and sensitivity treatment, and (iv) surfaces the causal and structural drivers behind diverse decarbonization pathways.

1. Integrating Machine Learning, Energy System Planning, and Policy Contexts.

The thesis occupies a genuinely interdisciplinary space by embedding machine learning not merely as a predictive layer but as an exploratory engine within a policy-aware planning framework. This integration respects spatiotemporal constraints of the underlying power system model while enabling the discovery of non-intuitive dependencies between policy levers (e.g., carbon pricing), technology deployment choices, and system-level outcomes. The framework supports answering both “what could happen” and “why it happens,” providing richer, more defensible guidance for strategy design under deep decarbonization.

2. Surrogate Modeling to Enable Massive Output-Space Exploration.

A deep neural network surrogate for the computationally intensive COPPER capacity expansion model lies at the core of the technical innovation. It collapses run times from many hours on high-end compute to milliseconds on commodity hardware while maintaining high fidelity. This acceleration makes feasible the simultaneous sampling of broad, high-dimensional input spaces and the generation of structured output datasets—permitting uncertainty, sensitivity, and pathway analyses at a scale and resolution that would be intractable with the base model alone. The surrogate’s efficiency also makes it realistic to embed into near–real-time decision-support or adaptive policy evaluation processes.

3. Output-Space–Centered Characterization of System Behavior.

A defining methodological contribution is the shift of analytical focus from isolated “optimal” outcomes to the comprehensive characterization of the output space. Through structured generation of large ensembles and the application of information-theoretic metrics (mutual information), rank correlations, and K-means feature importance clustering, the thesis uncovers system bifurcations, robust versus fragile pathways, and the principal

drivers of scenario divergence. This lens makes explicit the internal structure of plausible futures, filling a gap in traditional modeling which often stops at a small number of summary scenarios.

4. Extensive and Systematic Uncertainty and Sensitivity Analysis.

The thesis builds a disciplined foundation for uncertainty quantification by empirically identifying, expanding, and sampling realistic input parameter ranges—including carbon tax trajectories, capital cost and technology evolution uncertainty, demand growth, and capacity factors—using Latin Hypercube Sampling. The propagation of these deeply sampled uncertainties through the surrogate enables nuanced output variability characterization. In addition, the work conducts extensive sensitivity analysis (e.g., varying renewable capital costs and fuel prices) to test the stability of insights and to quantify how key assumptions shift the decarbonization pathways, thereby strengthening the robustness and credibility of recommendations.

5. Interpretable Communication via Structured Visualization.

High-dimensional outputs are distilled into interpretable forms through visualization techniques—cluster-weighted importance charts, dependency heatmaps, and ranked summaries—that translate complex interdependencies into actionable narratives. These tools bridge the gap between technical model output and policy/planning audiences, enabling scenario exploration and trade-off analysis without requiring deep immersion in the underlying mathematics or optimization machinery.

6. Regional (Provincial-Level) Pathway Elucidation under Uncertainty.

Extending beyond the national aggregate, the thesis adapts the surrogate and output-space methodology to capture provincial heterogeneity in demand growth, technology costs, carbon policy sensitivity, and transmission dynamics. This enables derivation of least-cost decarbonization pathways that recognize the federated structure of the electricity system, clarifying the differentiated roles of gas combined cycle, hydro, VREs, and transmission expansion across jurisdictions.

6.2.1 Key System-Level Insights

- Policy and cost levers—notably carbon taxation and wind capital costs—emerge as dominant in shaping emissions trajectories and the generation mix, highlighting where complementary support amplifies decarbonization impact.
- Gas combined cycle acts as a flexible backbone enabling high renewable integration, while hydroelectricity provides a stable, low-sensitivity anchor in many futures.
- Transmission expansion is tightly coupled to spatial variations in VRE capacity factors, underscoring the necessity of geographic integration to access high-quality renewable resource regions.
- Nuclear and diesel are de-emphasized across many plausible futures, suggesting caution in relying on them without substantial changes in cost or policy.
- Solar power, despite lower capacity factors, can exert outsized influence on scenario differentiation due to its temporal and locational characteristics, informing its strategic value.

6.2.2 Limitations

This work is careful not to overstate completeness. Primary limitations include:

- **Inherited assumptions from the base model.** The surrogate reflects structural simplifications in COPPER (e.g., continuous treatment of some capacities, approximated transmission, fixed capacity factor assumptions in some submodules). Updates to COPPER necessitate surrogate retraining to maintain alignment.
- **Surrogate interpretability.** While enabling large-scale exploration, the internal representations of the deep surrogate are less transparent than the underlying optimization; future work could pair it with hybrid physics-ML interpretability diagnostics or causal model attribution techniques.
- **Granularity and institutional realism.** Provincial-level analysis omits finer intra-provincial spatial constraints, land-use nuance, and decentralized stakeholder objectives, which could influence feasibility, equity, and implementation complexity.
- **Lack of endogenous feedbacks.** Key inputs—such as demand growth, policy responses, and technological learning—are treated exogenously; embedding dynamic feedback mechanisms (e.g., demand response to policy shifts or learning-curve-driven cost evolution) would improve realism.
- **Climate variability impacts.** The analysis assumes historical renewable capacity factor distributions; incorporating future climate projections and extreme event risk would better capture future supply-side uncertainty.
- **Policy evolution uncertainty.** Carbon pricing and regulatory regimes beyond current commitments are uncertain; systematic incorporation of policy-design uncertainty and scenario updating would bolster long-term robustness.

6.2.3 Broader Implications

The surrogate modeling and output-space analytical toolkit developed here is transferable beyond the Canadian case. Its low computational cost and structured uncertainty framing make it suited for embedding into operational decision-support systems, continuous policy stress testing, and adaptive planning in other jurisdictions facing the dual challenges of reliability and emissions reduction. By shifting practitioner attention from singular narratives to portfolios of plausible futures grounded in system structure, the framework promotes more resilient, informed, and strategic decarbonization planning.

6.2.4 Final Reflection

By combining machine learning acceleration, rigorous uncertainty/sensitivity quantification, high-fidelity system structure, and policy contextualization, this thesis establishes a new methodological foundation for energy transition analysis. It demonstrates that the value of modern data-driven tools lies not only in prediction but in exploration—revealing hidden systemic structure, identifying robust strategies across varied conditions, and

making complex decarbonization dynamics navigable for decision-makers. The insights produced here offer immediate relevance for Canada's electricity transition and provide a generalizable template for other systems grappling with deep uncertainty and ambitious climate objectives.

6.3 Future work

As discussed in chapter four, modeling frameworks inherent limitations. To address these limitations, we outline potential areas for further research and development:

1. **Improving Interprovincial Transmission Flows Representation:** The current model fixes interprovincial transmission flows. This limits the depiction of interactions between interconnected markets. Future research should focus on a more realistic representation. This would enable real-time energy transfers based on cost and demand.
2. **Improving National-Level Expansion Planning:** Enhancing accuracy requires moving beyond uniform constraints on wind and solar capacities. Geographical factors like terrain and urban landscapes should be considered. This will better represent renewable energy potential.
3. **Addressing Intra-Provincial Transmission Capacity Constraints:** The translation tool assumes fixed intra-provincial transmission capacities. This limits expansion planning accuracy. Future research should address this limitation in the COPPER model.
4. **Adapting to Evolving Decarbonization Policies:** Decarbonization policies at federal and provincial levels are changing. The surrogate model must be re-trained on updated data to align with new regulations. This ensures analyses stay relevant and support sustainability goals.
5. **Incorporating Uncertainties in Wind and Solar Capacity Factors:** Future research should include uncertainties in wind and solar capacity factors. This will improve the precision of power system modeling. It provides a more realistic assessment of renewable energy potential and its implications for the Canadian electricity system.

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7 Appendix

7.1 Appendix A: Models Validation

In this thesis, we ran the COPPER model to train the ML-based surrogate model. The validation section is split into two parts. Firstly, we validate the COPPER model using standard testing and validation methods [187], [188]. Then, we provide additional validation for the ML-based surrogate model.

7.1.1 COPPER

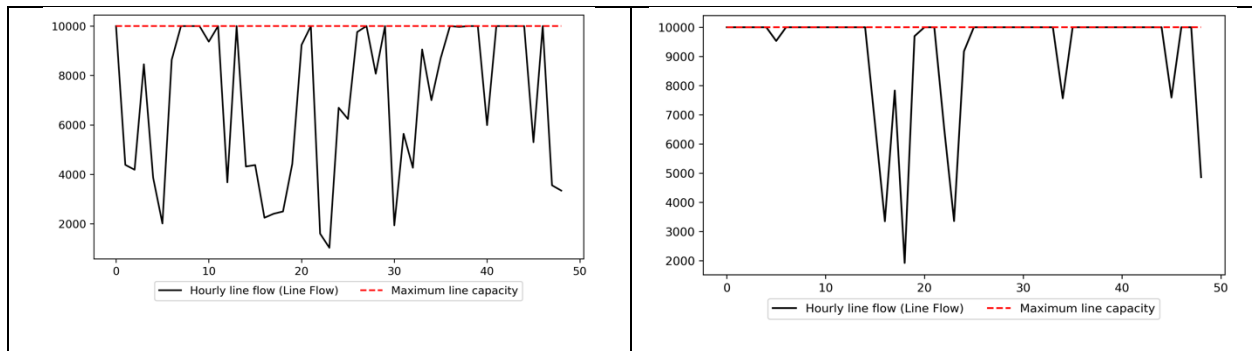
In this study, COPPER is used to project power system expansion while considering diverse decarbonization policy inputs and its original model documentation is available in [99]. The reliability of COPPER's results has been confirmed through comparisons with multiple studies related to Canada's power system. Arjmand et.al validated the core constraints of the COPPER and elaborated on its formulation and verified results by comparing to other studies [99].

COPPER's outcomes align with findings from other well-established capacity expansion planning studies in Canada such as the research by Dolter et al. [23], and Canada's Energy Future [189], the official annual energy report.

Further validation of the model will be discussed in upcoming subsections, including validation of couple of constraint validation and sensitivity analysis.

7.1.1.1 Validating constraints

1. Transmission capacity. Transmission is one of the main areas of focus in third and fourth chapter and results reveal its pivotal role in planning toward deep decarbonization. One crucial constraint guarantees that the flow through the interconnections never surpasses their specified nominal capacity. To ensure adherence to this constraint, a range of capacities for the same interconnection between British Columbia and Alberta are examined. Figure 29 illustrates the outcomes, confirming that the constraint is consistently met under various circumstances.



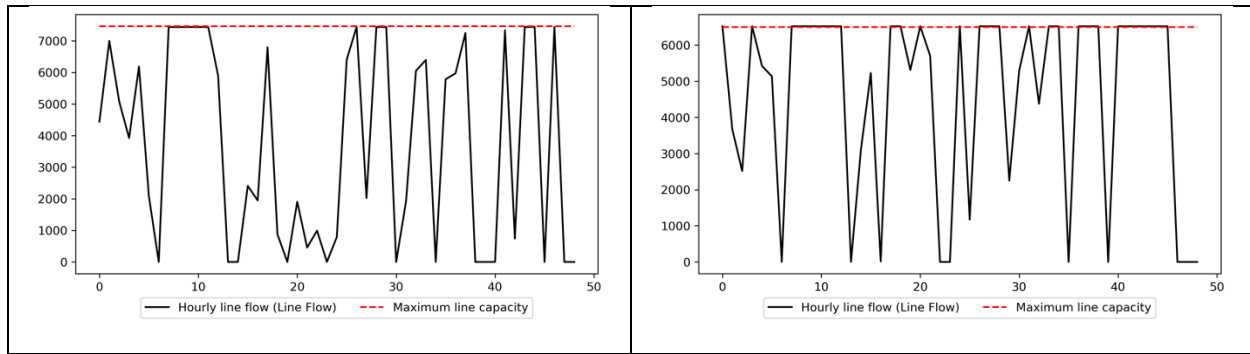


Figure 29 Hourly line flow compared to the line's maximum capacity

2. Hydroelectric is one of the focuses of third chapter. COPPER implements a standardized minimum generation constraint of 10% across all hydro capacity elements. The constraint's validation is conducted across diverse scenarios, as depicted in Figure 30, demonstrating its adherence in various conditions.

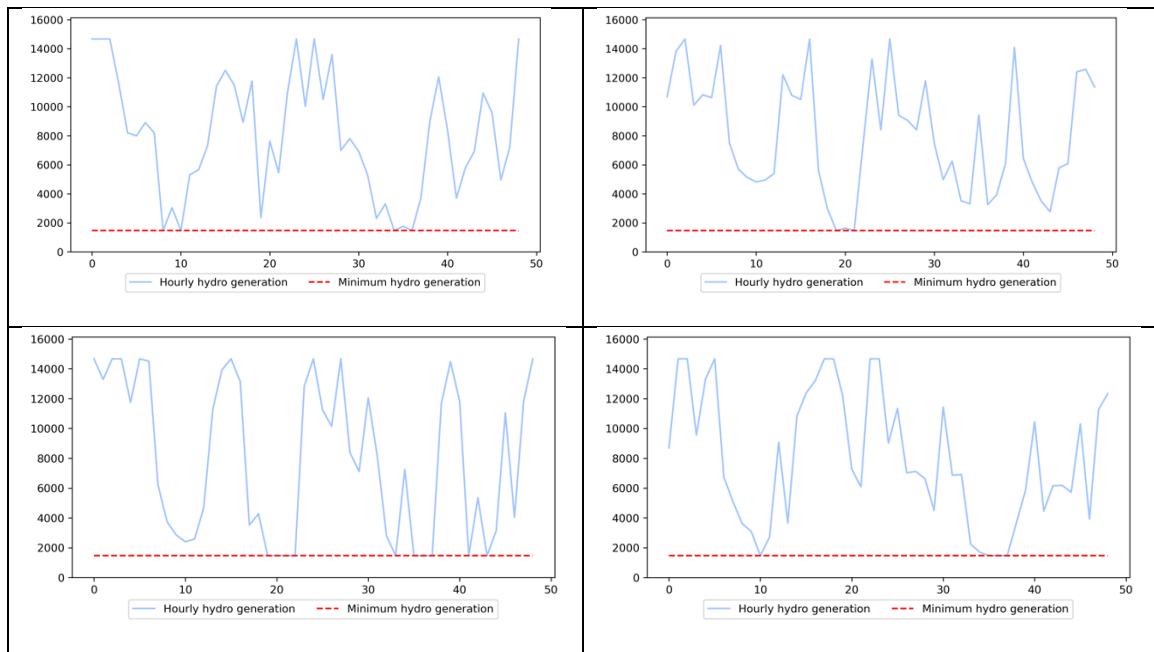


Figure 30 Hourly hydro output compared to minimum generation constraint

7.1.1.2 Sensitivity analysis

Carbon tax. Carbon tax as a policy tool in COPPER has a significant role in decarbonizing the power system and is modeled to represent current Canadian policies in place, it is one of the main policies considered in this study. The carbon tax policies are set to increase to up to \$170/ton by 2035 in a \$10/year increase. We run COPPER in the range that we had selected for training surrogate model which is set to have a range of \$0 to \$20 increase from 2020 to 2050 to analyze the sensitivity of different outputs to this change in input. Results are shown in Figure 31 for emitting capacities, emissions, wind capacity, and solar capacity.

As the annual carbon tax increase, both the capacities associated with emissions and the actual emissions exhibit a consistent negative correlation. This aligns with the expected system behavior, wherein the model avoids expanding and operating emitting capacities in order to minimize costs as carbon expenses rise.

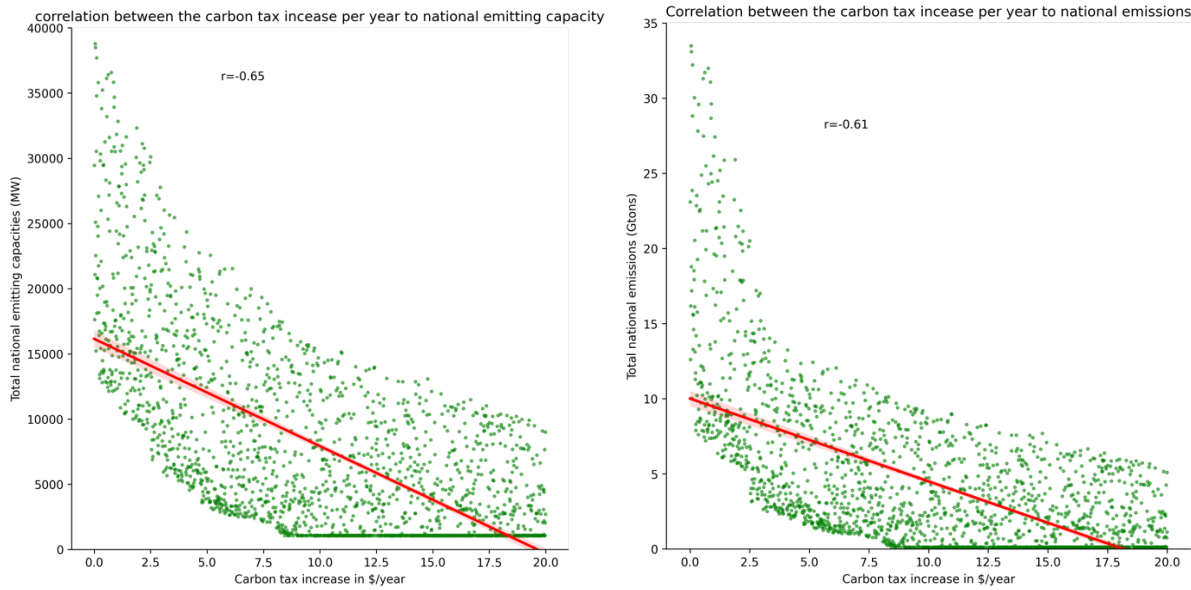


Figure 31 Correlation between a carbon tax increase and emitting capacities and emissions

As the annual tax rises, wind capacities increase while emitting capacities decrease. Wind investment costs vary, impacting this correlation. Solar capacities, however, show slight negative growth with higher carbon taxes, discussed further in Chapter four. In summary, the model prefers wind over solar due to lower future costs, higher potential in Canada, and closer proximity to the grid, leading to reduced transmission expenses.

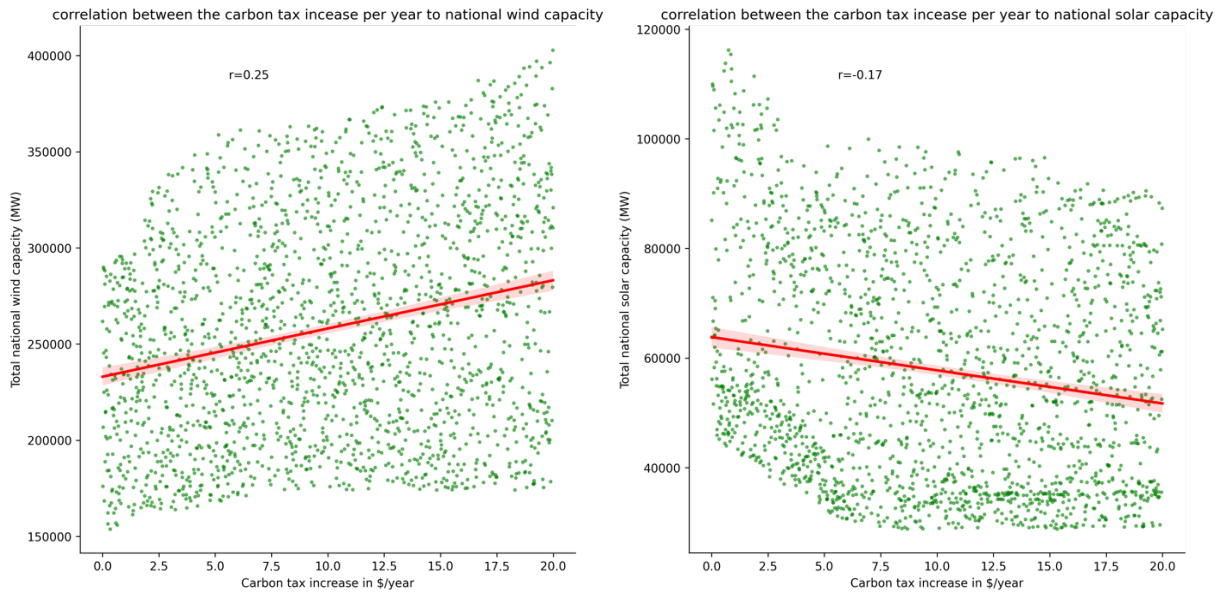


Figure 32 Correlation between a carbon tax increase and wind and solar capacities

One primary constraint within COPPER requires that supply meets the demand during sample hours. Consequently, the model must exhibit a correlation between supply and demand as load curves change. The generation capacity should demonstrate sensitivity to shifts in demand, dependent on the equilibrium between supply and demand. The findings are illustrated in Figure 33, demonstrating a highly significant positive correlation between the total installed capacity and the demand growth rate from 2018 to 2050. This analysis provides additional validation for the model, confirming its adherence to the demand and supply balance constraint.

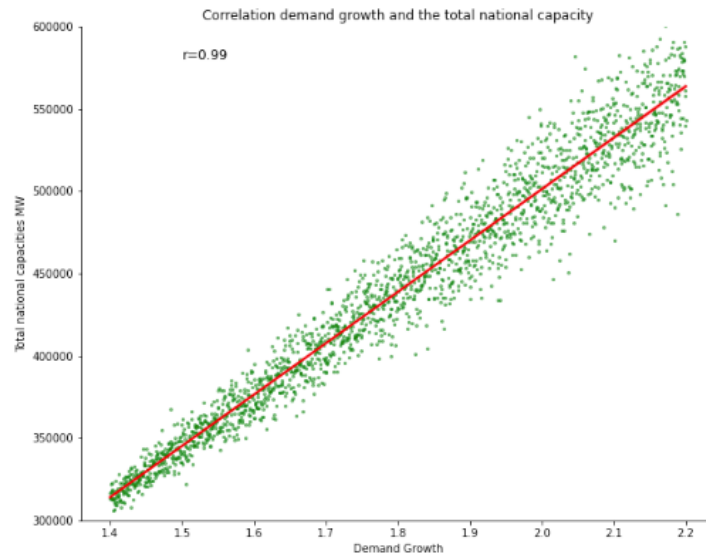


Figure 33 Correlation between increasing demand with the total generation capacity

7.2 Appendix B: Loss curves and clustering plots

As extensively detailed in this thesis, we employed a neural network with residual blocks to construct a surrogate model based on the COPPER framework. Regression plots, R-squared values for the test dataset, and Mean Squared Error (MSE) loss are presented in each chapter. Figure 34 depicts the loss curves for the selected model in chapter two as a sample to show how we monitored the loss, which demonstrates that the model neither overfits nor underfits the data.

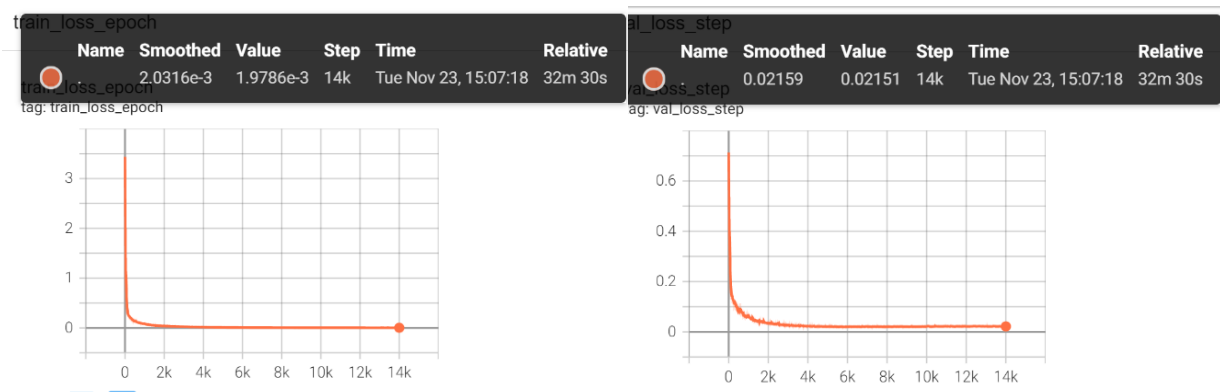


Figure 34 Loss Curves

7.3 Appendix C: Data and source codes

Data sources are all listed in the chapters and can be accessed by request. All models, analysis, post-process, and visualization codes can be accessed through their respective repositories and websites as presented in the below table:

<i>No.</i>	<i>Repository name</i>	<i>Repository address</i>
1	COPPER model	https://gitlab.com/McPherson/copper
2	Model development and Visualization	https://github.com/ZahraJahangiri/DL_COPPER
3	The raw data for training the ML model	available on the SESIT website (https://sesit.cive.uvic.ca/) Under Zahra Jahangiri's profile, with a direct link at https://sesit.dev/zahra/download