Appendix
Regionalisation in high share renewable energy system modelling

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***Abstract*—This document corresponds to the appendix of the paper *Regionalisation in high share renewable energy system modelling* by Schnidrig et al. in redaction, and is based on the Master thesis of Amara Slaymaker 2021, giving additional information about the methodology, data used and assumptions made.**
This Appendix is structured in three parts. First the methodological details of the energy system model *EnergyScope* are given, followed by (ii) the clustering method details with data sources and results and (iii) additional results and validation of the model.

***Index Terms*—Appendix, energy, optimisation, renewable, system, transition**

I. Energy System Modelling

A. *EnergyScope*

B. *Regionalisation*

II. Region Charactersiation

A. *Clustering*

The map of Canada was first divided into smaller subregions defined by Canada's Census Subdivisions (CSDs) (figure **??**). Although the CSDs are still a form of political region definition, these are simply used as a basis for assigning attributes. As can be seen in figure **??**, the CSDs are much smaller than the provinces, and there would be too many CSDs to model all of them in an energy system.

The value of each selected attribute was determined and assigned to each CSD based on geospatial data analysis (II-B). The CSDs belonging to the same cluster are then modelled as a single cluster/region within the ES-R DG model.

Once the value of each attribute was determined for each CSD, the attributes were prepared for clustering by scaling using the min max method, which normalizes the data between 0 and 1 as follows:

$$X_i^{'} = \frac{X_i - X_{min}}{X_{max} - X_{min}} \quad (1)$$

EnergyScope 2.0 project within Swiss Federal Office of Energy funding.

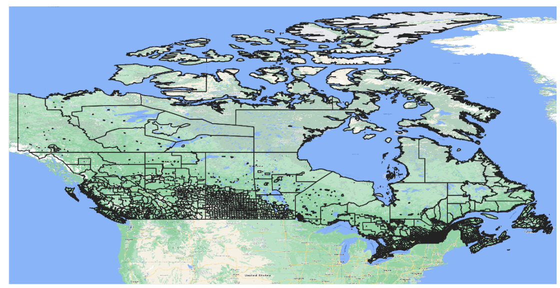

Fig. 1. Census Subdivisions

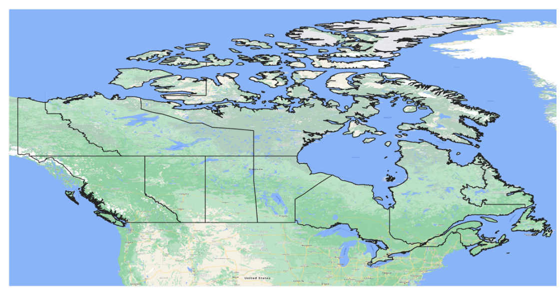

Fig. 2. Provinces of Canada

where $X_i^{'}$ is the scaled value i of attribute X, X_i is the original value, and $X_{m}in$ and $X_{m}ax$ are the minimum and maximum values of attribute x, respectively.

Following this, the k-means clustering algorithm was applied. The k-means algorithm solves the following optimization problem:

$$min \sum_{j=1}^{k} \sum_{i=1}^{n} \| x_i^{(j)} - c_j \|^2 \quad (2)$$

which is where k is the number of clusters, n is the number of cases, c_j is the centroid of cluster j and $x_i^{(j)}$ is case i in cluster j.

The number of clusters must be selected by the algorithm user. In order to select the number of clusters, following indicators were considered for different values of cluster number k:

The total sum of errors squared (SES):

$$SES = \sum_{j=1}^{k} \sum_{i=1}^{n} \| X_i^{(j)} - C_j \|^2 \tag{3}$$

The average error squared (AES):

$$AES = \frac{1}{n} \sum_{j=1}^{k} \sum_{i=1}^{n} \| X_i^{(j)} - C_j \|^2 \tag{4}$$

The average relative error (ARE):

$$ARE = \frac{1}{n} \sum_{j=1}^{k} \sum_{A}^{a=1} \sum_{i=1}^{n} \frac{|x_{i,a,j} - c_{a,j}|}{x_{i,a,j}} \tag{5}$$

The average inter-cluster distance (AICD):

$$AICD = \frac{1}{k^2} \sum_{j=1}^{k} \sum_{i=1}^{k} \| c_i - c_j \|^2 \tag{6}$$

The following section discusses the results of the k-means clustering method applied to the selected set of geographic and demographic attributes of Canada, which was used to define a new set of regions based on these attributes.

The k-means clustering algorithm was tested for 1-25 clusters, and the resulting distortion (sum of normalized errors squared), as well as the percent improvement in distortion for each increase in cluster number (figure 3) was analyzed. As can be seen, the distortion improves significantly when going from 1 to 3 clusters, and remains above 10% improvement with each added cluster until 5 clusters. ... A number of clusters between 5 and 12 is thus likely ideal, as with less than 5 the error is very high and above 12 the decrease in error is small and may not be worth the increased computational time required. Here it can be seen that increasing from 5 to 10 clusters significantly reduces the errors (by more than 20%) while minimally reducing the inter-cluster distance (by less than 10%).

B. Geospatial Data Processing

As mentioned, the geospatial data used for cluster definition was processed using the geographical information systems tool QGIS. The GIS data and sources used for determining the attributes discussed above are listed in table II.

The GHI and wind speed data were available for environmental weather stations spread across Canada. Each CSD was assigned the average GHI and wind speed values based on the closest stations. The solar c_p was calculated from the GHI as:

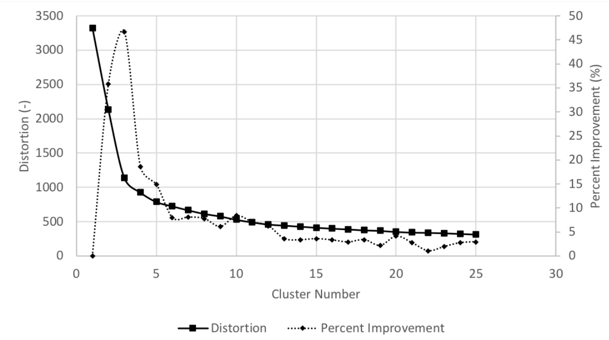

Fig. 3. Cluster Number vs Distortion for K-Means Clustering

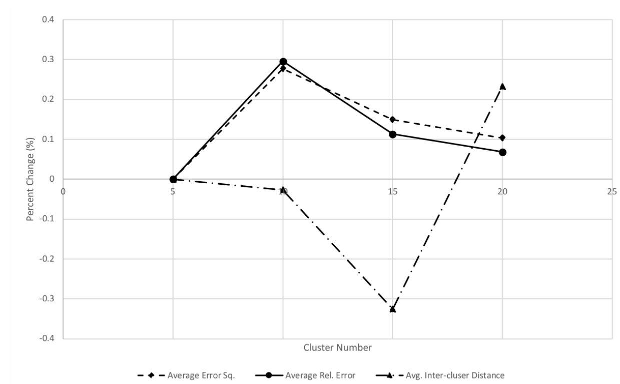

Fig. 4. Cluster Number vs Average Errors and Inter-Cluster Distance

TABLE I
CLUSTER CENTROIDS

Cluster	Description
Vancouver	Inhabited area with medium grid distance and high wind and hydro potentials
Montréal	Urban area with agricultural potential close to the grid with medium wind and high solar potentials
Grande Prairie	Sparsely inhabited agricultural area close to the grid with high solar potential
National Park	Agriculture area near the grid with high solar, wind and hydro potentials
Albertville	Urban area with medium grid distance and high hydro potential and wind potential
Winipeg	Agricultural area near the grid with medium solar, wind and hydro potentials
Inuvik	Sparsely inhabited area far from the grid with high wind potential
Calgary	Agricultural area near the grid with high wind potential
Edmonton	Sparsely inhabited area far from the grid with high wind and hydro potential
Ottowa	Urban area near the grid with medium solar, wind and hydro potentials

$$c_{p,solar} = \frac{GHI_{avg} \frac{kW}{m^2}}{1000 \frac{kW}{m^2}} \tag{7}$$

The wind c_p was calculated using the approximation in [1], which relates the capacity factor to the wind speed (μ_v) in m/s , turbine rotor diameter (D) in m and turbine rated power

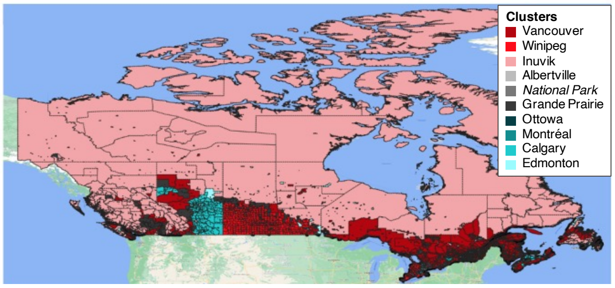

Fig. 5. Clustered ecumene areas of Canada

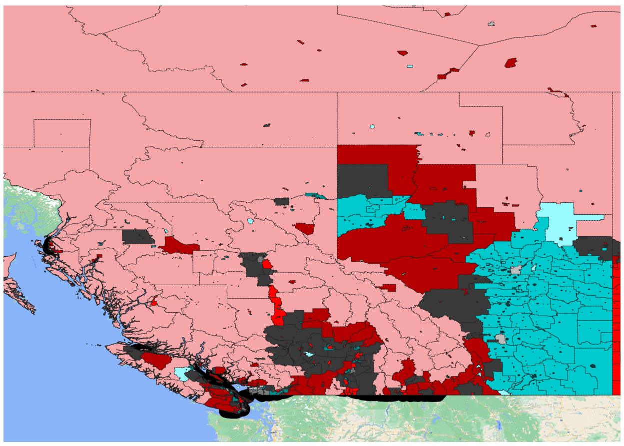

Fig. 6. Clustered ecumene areas of Canada - zoom Southern Quebec and Atlantic

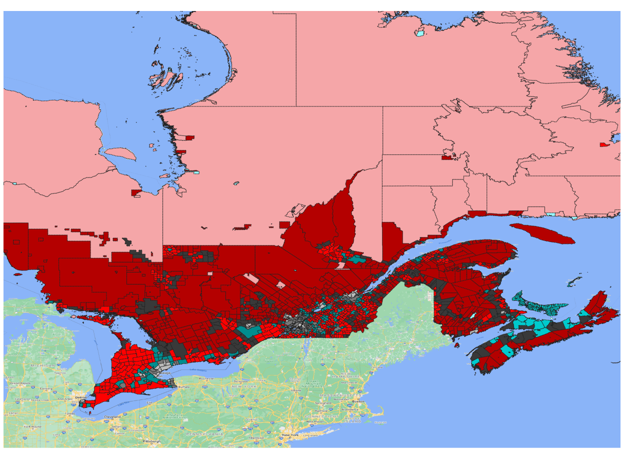

Fig. 7. Clustered ecumene areas of Canada - zoom Alberta and British Columbia

(P_r) in kW. A rotor diameter of 110m [2] and a rated power or 2MW [3] were assumed.

$$c_{p,wind} = (1 - 0.087)\{tanh(\frac{0.087 \cdot \mu_v^2}{2\pi \cdot (1 + (P_R/D^2)) + P_R/D^2} - \frac{0.087}{2\pi \cdot (1 - (P_R/D^2)) \cdot \mu_v})\} \quad (8)$$

First, total existing hydro capacity (MW) of each CSD was determined based on the GIS data. Canada's additional, undeveloped hydro potential (as defined in [4]) was assumed to be distributed proportionally to existing hydro potential. ... It should be noted that this assumption is a limitation of the cluster definition method, as there may be hydro potential in areas which currently have no developed hydro plants - however, GIS regarding the distribution of undeveloped hydro potential was not available. The hydro c_p was determined for each province based on data regarding annual installed capacity [5] and generation [6]. This was achieved using the distance calculation tool in QGIS, which calculates the distance from the center of each cluster to the closest network point. The percentage of each CSD's area corresponding to urban, agricultural and ecumene areas was determined using the CSD map data, as well as the ecumene maps provided by Statistics Canada and Natural Resources Canada. The area available for wind and solar was calculated based on the data regarding the urban and agricultural land area, as well as the land cover type. ... Of the other area, it was considered that agricultural area was 100% available for wind development, and 20% available for solar [7]. Finally, it was considered that an additional area of 13 m^2/capita was available for development of rooftop solar installations, based on [8] which analyzed the per capita area suitable for rooftop PV in Ontario, Canada. Using these factors, the total value and percentage of each CSD's area available for wind and solar technology was calculated.

TABLE II
GEOSPATIAL DATA - DATA SOURCES

Geospatial Data	Unit	Source
Average annual GHI	kW/m^2	Government of Canada [9]
Average annual Wind Speed	m/s	Government of Canada [9]
Land Cover Type	-	Government of Canada [10]
Transmission Network	-	Natural Resources Canada [11]
CSD Area and Population	-	Statistics Canada [12]
Hydro Plants	-	Natural Resources Canada [11]
Urban Ecumene	-	Statistics Canada [13]
Agricultural Ecumene	-	Statistics Canada [14]
Extended Ecumene	-	Natural Resources Canada [13]

III. CASE STUDIES

A. 2018 Canadian Energy System - ES-R Canada

The 2018 Canadian energy system was selected as the reference system to use for validation of the ES-R Canada model as data regarding the energy demands and energy generation of this system are well documented and can be used for comparison in order to validate that the model is functioning as expected.

1) End-Use Demands: This database provides end-use energy demand data for five sectors - residential, commercial, industrial, transportation and agriculture - and for different regions (provinces, territories, or groups in some cases a group of provinces and/or territories). In order to relate the data available in this database to the main sectors and demand types that describe the EUDs within the ES-R Canada model, the following additional assumptions were made.

Residential

For the residential sector, data was provided according to the following categories: space heating, water heating, appliances, lighting and space cooling. A small portion of this demand is for natural gas - for example for use in gas cooking stoves - however, this represents a small portion and was neglected. Space cooling demand was neglected, as cooling technologies are not yet integrated into ES and space cooling represents a small percentage of the total residential energy demand in each province (between 0 and 1.62% in every province and territory except for Ontario and Manitoba, where it represents 4.18% and 4.10% respectively).

Data was available for each province, however the data regarding the three territories (YT, NT, NU) was grouped together.

$$EndUseDemand_{rc,i} = EndUseDemand_{rc,territories} \cdot \frac{Demand_i}{\sum_{j=1}^{3} Demand_j} \quad (9)$$

where $EndUseDemand_{c,i}$ is the end use demand of territory i in residential category rc, $EndUseDemand_{c,territories}$ is the total end use demand of all territories in residential category cc, $Demand_i$ is the total annual energy demand (excluding industrial energy demand) of territory i and $Demand_j$ is the total annual energy demand (excluding industrial energy demand) of territory j.

For the commercial sector - referred to as the services sector in ES - data was available for the following categories: space heating, water heating, auxiliary equipment, auxiliary motors, lighting, space cooling and street lighting. It was specified in the database that the auxiliary motors consumed only electricity, therefore this demand was attributed to electricity demand [15]. Finally, the auxiliary equipment demand was further analyzed according to energy source and further broken down into electricity, which was therefore attributed to electricity demand, and natural gas, coal and propane, which was attributed to high temperature heating demand.

Data for the four Atlantic provinces (NL, NB, NS, PE) was grouped together, and data for BC and the three territories (YT, NT, NU) was grouped together.

$$EndUseDemand_{cc,i} = EndUseDemand_{cc,group} \cdot \frac{GDP_{services,i,2018}}{\sum_{j=1}^{n_{group}} GDP_{services,j,2018}} \quad (10)$$

where $EndUseDemand_{sc,i}$ is the end use demand of province or territory i in services category cc, $EndUseDemand_{sc,group}$ is the total end use demand of the group in services category cc, $GDP_{services,i,2018}$ is the GDP of the services sector of province or territory i in 2018, $GDP_{services,j,2018}$ is the GDP of the services sector of province or territory j, and n_group is the number of provinces or territories in the group. The GDP of the services industry was obtained from Statistics Canada [16].

Industry For the industrial sector, data was available either per industry (for example pulp & paper, construction, cement, etc.) or per energy source (for example electricity, natural gas, coal, fuel oil). Therefore, additional assumptions were made to divide this into the ES EUD types of electricity, lighting, high temperature heating, space heating, and water heating.

For the electricity energy source, it was assumed that 6% of the total electricity was lighting demand[17], and that the remaining 94% was electricity demand. ... In order to separate this heating demand further into high temperature (HT), space heating (SH) and water heating (HW) demand, the percentages in table III. The percentages were approximated according to the findings of Naegler et al.[18]. Where there were differences between the industry types found in Canada's energy demand database and those studied by Naegler et al., the following assumptions were made.

TABLE III
HEATING DEMAND IN INDUSTRY - HIGH TEMPERATURE, SPACE HEATING AND WATER HEATING DEMAND PERCENTS OF TOTAL HEATING DEMAND, ACCORDING TO INDUSTRY TYPE [18]

Industry Category	HT (%)	SH (%)	HW (%)
Construction	84.00	13.60	2.40
Pulp and Paper	97.50	2.50	0.00
Smelting and Refining	83.00	14.96	2.04
Petroleum Refining	97.50	2.50	0.00
Cement	97.50	2.50	0.00
Chemicals	82.00	18.00	0.00
Iron and Steel	97.50	2.50	0.00
Other Manufacturing	84.00	13.60	2.40
Forestry	87.00	13.00	0.00
Mining, Quarrying, Oil and Gas Extraction	96.00	4.00	0.00

In terms of groups, similarly to the services sector, the industry sector data had two groups - Atlantic provinces (NL, NB, NS, PE) and BC and Territories (BC, YT, NT, NU). The grouped data was allocated as follows:

$$EndUseDemand_{isc,i} = EndUseDemand_{isc,group} \cdot \frac{GDP_{industry_{cat},i,2018}}{\sum_{j=1}^{n_{group}} GDP_{industry_{cat},j,2018}} \quad (11)$$

where $EndUseDemand_{isc,i}$ is the end use demand of province or territory i in industrial energy demand of energy source category isc, $EndUseDemand_{isc,group}$ is the total end use demand of the group in industrial energy source category isc, $GDP_{industry_{cat},i,2018}$ is the GDP of the relevant industry category of province or territory i in 2018, $GDP_{industry_{cat},j,2018}$ is the GDP of the relevant industry category of province or territory j, and n_group is the number of provinces or territories in the group. ... It should be noted that for the energy source natural gas, n_group for the BC and Territories group was taken as 3 and included BC, YT and NT. NU was excluded from the group as NU does not consume any natural gas [19].

Transportation The energy demand for transportation was available for several transportation types, including both passenger transportation modes (car, passenger light trucks, motorcycles, school buses, urban transit, inter-city buses, passenger air, passenger rail and off-road) and freight transportation modes (freight light trucks, freight medium trucks, freight heavy trucks, freight air, freight rail, and marine). For the purposes of this thesis, air transportation (both freight and passenger), marine transportation and off-road transportation were excluded from the analysis. The database also provided the energy intensity of each transportation mode, in terms of MJ/pkm (passenger transport) or MJ/tkm (freight transport). This data was therefore used to convert the demand into passenger-kilometers (pkm) or tonne-kilometers (tkm) for ES. The transportation sector had one data group - BC and Territories (BC, YT, NT, NU).

$$EndUseDemand_{tm,i} = EndUseDemand_{tm,group} \cdot \frac{Pop_{i,2018}}{\sum_{j=1}^{n_{group}} Pop_{j,2018}} \quad (12)$$

where $EndUseDemand_{tm,i}$ is the end use demand of province or territory i for transportation mode tm, $EndUseDemand_{tm,group}$ is the total end use demand of the group for transportation mode tm, $Pop_{i,2018}$ is the population of province or territory i in 2018, $Pop_{j,2018}$ is the population of province or territory j, and n_group is the number of provinces or territories in the group. ... Data was provided on a quarterly basis, therefore the population of 2018 was taken as the average population over the four periods.

Agriculture The agricultural end use demand data was broken down into non-motive energy demand (with energy resources electricity, natural gas, light fuel oil, kerosene, heavy fuel oil, propane and steam), and motive energy demand (with energy resources motor gasoline and diesel fuel oil).

Regarding the motive energy demand, it was assumed that all of this demand was linked to transportation, and this was therefore attributed to freight transportation demand. The energy demand provided was converted into tonne-kilometers (tkm), the unit used to describe freight transportation demand, using the average energy intensity (in terms of MJ/tkm) of freight trucks (light, medium and heavy) provided in the transportation section of the database, as discussed above. Regarding the non-motive energy demand, it was assumed that 4% of the electricity source demand was lighting demand, with the remainder being electricity demand [20]. It was further assumed that the energy demand from all remaining sources was heat demand, with 10% being water heating demand and the remainder being space heating demand [20].

Again, the agricultural sector data had two groups - Atlantic provinces (NL, NB, NS, PE) and BC and Territories (BC, YT, NT, NU).

$$EndUseDemand_{ac,i} = EndUseDemand_{ac,group} \cdot \frac{GDP_{agriculture,i,2018}}{\sum_{j=1}^{n_{group}} GDP_{agriculture,j,2018}} \quad (13)$$

where $EndUseDemand_{ac,i}$ is the end use demand of province or territory i in agriculture energy source category ac, $EndUseDemand_{ac,group}$ is the total end use demand of the group in agriculture energy source category ac, $GDP_{agriculture,i,2018}$ is the GDP of agriculture of province or territory i in 2018, $GDP_{agriculture,j,2018}$ is the GDP of agriculture of province or territory j, and n_group is the number of provinces or territories in the group. The GDP data was obtained from Statistics Canada [16]. Again, NU was assumed to have no demand for natural gas.

2) Resources: Specific values of availability were calculated for the following ES resources: waste, wood, dry wood, wet biomass and biogas.

Availability The availability of waste in terms of kg/province/year was determined from [21] for 2016. Increase in waste availability (for the year 2018) was assumed to be equivalent to population growth. An average value of 10 MJ/kg[22] was used to determine the annual availability in terms of GWh/year.

The availability of residual biomass resources from foresty, crop agriculture and animal agriculture were determined from [23] for the year 2001 in terms of GWh/year. The increase in availability for the year 2018 was considered equivalent to the GDP growth between 2001 and 2018 of the forestry and logging, cop production and animal and aquaculture industries respectively. The availability from crop and animal agriculture was considered wet biomass. Of the availability from forestry, 57% was considered wood and the remaining 43% was considered dry wood (assuming Canada has a similar wood to dry wood ratio to for Switzerland, where this value was available from adaptations of the ES model).

As determined by the report, 68% of the biogas potential comes from agriculture - therefore, the biogas potential per province was assumed to be proportional to the agricultural GDP (accounting for both crop production and animal and aquaculture).

TABLE IV
RESOURCE AVAILABILITY DATA SOURCES

Resource	Source
Waste	Environmental & Climate Change Canada [21]
Biomass	BIOCAP Canada Foundation [23]
Biogas	Biogas Association [24]

Operating Costs

A summary of the operating costs used in the model can be found in table V. As resource prices are not fixed and depend on market variations, values within the fluctuation range were selected. Generally, prices in the higher range were selected.

TABLE V
RESOURCE OPERATING COSTS

Resource	Cost (CAD/kWh)	Source
NG	0.011	[25]
LFO	0.037	[25]
Gasoline	0.14	[26]
Diesel	0.13	[26]
Coal	0.011	[27]
Wood	0.0016	[28]
Electricity Import	0.040	[29]
Electricity Export	0.039	[29]
Biogas	0.18	[28]
H_2	0.06	[30]

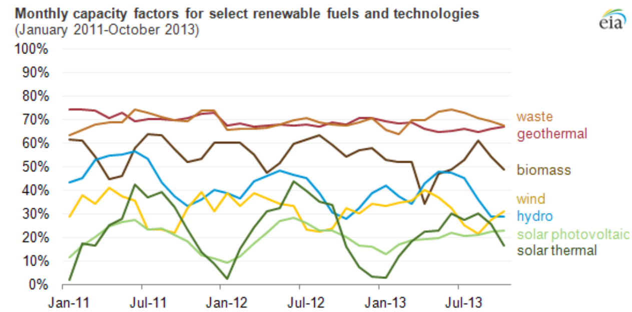

Fig. 8. Monthly Capacity Factors of Renewable Fuels and Technologies [34]

Technologies

Technology potentials were considered for renewable energies - including geothermal, solar, wind, hydro and solar - as the potential of these technologies is variable in terms of both time and space.

...The study also included a detailed analysis of the potential monthly generation at various wind sites This data was used to determine the capacity factor of each province in each month, which was taken as an average of all the wind sites within a given province included in the study. The wind energy potential of the Northwest Territories from [31] was used, and the other two territories (Yukon and Nunavut) were assumed to have the same potential as the Northwest Territories. The capacity factors were considered to be the same as that of their nearest province - Quebec in the case of Nunavut, Alberta in the case of the Northwest Territories, and British Columbia in the case of Yukon.

...First, the rooftop potential for each province was calculated assuming an area of 13 m^2 per capita [8], and the population of each province [32]. ... The potential was then calculated assuming a solar radiation of 1 kW/m^2, and a solar thermal efficiency of 30% [33]. For solar PV, the total urban area (already accounted for with the rooftop PV assumption), as well as the farm areas, and protected areas and forest areas were subtracted from the total province area. ... The potential was the calculated from the total land area, assuming again a solar radiation of 1 kW/m^2 and a solar PV efficiency of 20%.

...The capacity factor for solar PV was determined based on environmental weather station data which provided hourly GHI values (kW/m^2) [9]. ... The capacity factor for solar PV was used to determine a reasonable assumption for the capacity factor of solar thermal based on figure 8, where it can be seen that the capacity factor is almost double that of PV in the summer months, and almost half of that of PV in the winter months.

The installed and potential hydro capacity for each province was provided by [4]. As this data was not divided between river and dam hydro (as in ES), an review of existing hydro installations in each province was performed in order to determine the proportion of river versus dam hydro. The new hydro potential was assumed to follow the same proportions.

The monthly capacity factor of hydro for each province was determined based on data regarding the installed capacity [5] and monthly generation [6]. As this data was not separated into river and dam hydro, the following assumption was made. The calculated values were used for the c_p of both river and dam hydro for existing hydro technologies. For new hydro technologies, the monthly c_p of Alberta was taken for new dam hydro and the monthly c_p of Saskatchewan was taken for new river hydro, as these provinces have almost exclusively dam and river hydro respectively, and are therefore considered representative.

3) Energy System 2018 Parameters and Constraints: In order to model the 2018 Canadian energy system, additional constraints and parameters were specified in order to re-create a modelled system close to the actual one.

For electricity, the total electricity generation by each resource in 2018, as in [35], was used to determine the percentage contribution of each resource to the total electricity demand. For heating, the total use of each resource was available from [15] which was again used to determine the percentage contribution of each resource to the total heating demand.

$$\sum_{n_{j,i}} \sum_{t} F_{t(n,t,r)} \cdot t_{op(t)} \cdot layers_{in,out(n,i)} \leq f_{maxperc_{j,i}} \cdot \sum_{x_j} \sum_{t} F_{t(x,t,r)} \cdot t_{op(t)} \cdot layers_{in,out(x,i)} \tag{14}$$

$$\sum_{n_j} \sum_{t} F_{t(n,t,r)} \cdot t_{op(t)} \cdot layers_{in,out(n,i)} \geq f_{minperc_{j,i}} \cdot \sum_{x_j} \sum_{t} F_{t(x,t,r)} \cdot t_{op(t)} \cdot layers_{in,out(x,i)} \tag{15}$$

where $n_{j,i}$ is the set of conversion technologies n which generate layer i from layer j, $layers_{in,out(n,i)}$ is the amount of layer i generated per kW of unit n utilized, $x_{j,i}$ is the set of all conversion technologies which generate layer i, and $f_{minperc_{j,i}}$ $f_{maxperc_{j,i}}$ are the maximum and minimum percentages of layer i generated from layer j. $f_{minperc_{j,i}}$ $f_{maxperc_{j,i}}$ are defined based on the percentages calculated previously, $\pm 5\%$.

...For transportation, data regarding the use of specific transportation technologies was available from [15]. ... The end use types defined in ES for transportation include private passenger mobility, public passenger mobility, road freight mobility and train freight mobility. The ES parameters $f_{minperc_x}$ $f_{maxperc_x}$, which represent the minimum and maximum share of a given technology within its end use type, was defined based on the calculated percentages $\pm 5\%$.

...Additional parameters specific to the 2018 system include the maximum and minimum shares of public transportation (within passenger transportation) and maximum and minimum shares of train freight transportation (within freight transportation), which were again calculated based on data from [15]. The maximum and minimum shares of district heating networks (DHNs) (within low temperature heating) were set to 0.1 and 0 respectively, as the share of heating capacity provided by DHN technologies was reported as less than 7% [36]. The maximum and minimum shares of off-grid electricity demand (within electricity demand) were determined from the remote communities energy database [37].

...Given that the initial values were developed for Switzerland, and transportation behaviour is quite different in Canada due to the differences in transportation network, distances and population density, these values are impacted.

B. 2050 Canadian Energy System - ES-R H_2

Following validation of the ES-R Canada model, the 2050 energy system was modelled using ES-R H_2. Modelling of the energy system in 2050 requires the extrapolation and modification of certain parameters and constraints.

1) End-Use Demands: The end uses demands for 2050 were extrapolated from those determined for 2018 according to projections for population and GDP growth for Canada.

The projection for population growth was taken from Statistics Canada's medium growth (M1) scenario, which projects a population of 48.76 million in 2050[38]. Based on this, the percent increase was calculated as:

$$\%_{increase,pop} = \frac{Pop_{2050} - Pop_{2018}}{Pop_{2018}} \tag{16}$$

The projection for GDP growth was taken from PwC's *The World in 2050* report, which projects that Canada will reach a GDP of 3.1 trillion USD_{2016} by 2050, compared to a GDP of 1.5 trillion USD_{2016} in 2016 [39]. Based on this, an annual growth rate, *r*, was calculated assuming constant annual growth, as follows:

$$GDP_{2050} = GDP_{2016}(1 + r)^{(2050-2016)} \tag{17}$$

According to this growth rate, the 2018 GDP in USD_{2016} was calculated and from this, the overall increase from 2018 to 2050 was determined:

$$GDP_{2018} = GDP_{2016}(1 + r)^{(2018-2016)} \tag{18}$$

$$\%_{increase,gdp} = \frac{GDP_{2050} - GDP_{2018}}{GDP_{2018}} \tag{19}$$

Based on this, the end use demands for 2050 were calculated from the reference 2018 demands, where household, services, and passenger mobility demands were multiplied by $\%_{increase,pop}$ and the industry (including the demands for ammonia and steel), agriculture and freight mobility demands were multiplied by $\%_{increase,GDP}$ in order to obtain the values for 2050.

As mentioned above, the ES-R H_2 model also includes the demand for steel and ammonia. The data sources used for the demand for steel and ammonia production in Canada in 2018 can be seen in table VI. The data regarding production for the entire country was found, and distributed on a provincial level according to the GDP of the relevant industry (chemicals for NH_3, iron and steel for steel).

TABLE VI
CANADIAN AMMONIA AND STEEL DEMAND IN 2018 - DATA SOURCES

Parameter	Source
NH_3 Production (Canada)	Statistics Canada [40]
Chemicals Industry GDP (Provincial)	Statistics Canada [16]
Steel Production (Canada)	ITA [41]
Iron & Steel Industry GDP (Provincial)	Statistics Canada [16]

2) Technologies: The costs of wind and solar PV were updated according to [42]. Multiple scenarios of the price of PV and wind costs are presented - the more conservative reference scenario was selected.

...Given that as of 2018, Canada's freight trains are entirely diesel operated and the line is not at all electrified, as well as considering the differences in network and distances within the transportation system as discussed previously, there was a need to update the freight train data in order to model the potential of electrifying transport in 2050. Three electrical freight train technologies were added - overhead line electrified (OLE), fast charging battery electric and full battery electric. The efficiencies and costs were determined from a study regarding the electrification of train lines in Norway and the US [43]. The US parameters were taken, assuming that this is comparable to the case of Canada.

3) Energy System 2050 Parameters and Constraints: For the 2050 energy system, the maximum share of freight was set to 0.80 for each province, and the maximum share of public transportation was set to 0.30 for each province (in both cases, a value was selected which is slightly higher than province with the maximum value in the 2018 system).

Although the minimum and maximum shares of specific technologies are not constrained for the 2050 model, as the goal is to identify the optimal technologies for the system, a constriant is imposed on the maximum penetration of VREs (including wind and PV) in the grid.

$$\sum_{t}(F_{t(PV,t,r)} + F_{t(Wind,t,r)}) \cdot t_{op(t)} \leq 0.7 \cdot \sum_{t}\sum_{m} F_{t(m,t,r)} \cdot t_{op(t)} \cdot layers_{in,out(n,elec_{grid})} \quad (20)$$

where m is the set of all technologies generating on-grid electricity.

C. 2050 Canadian Energy System - ES-R DG Model

In general, the parameters and modelling considerations for the 2050 system are the same as described previously, unless otherwise stated below.

1) Technologies: As discussed previously, the geospatial data analysis and clustering process led to the definition of the parameters including cluster area and percent area available for wind and solar developments. Regarding solar, the overall potential (in terms of GW) was calculated using the same method described previously, assuming a solar irradiation of 1 kW/m^2 and efficiencies of 20% and 30% for solar PV and solar thermal respectively. For wind, a rated turbine power of 4MW/km^2 was assumed [3].

The capacity factors of wind, solar and hydro determine for each cluster were average annual values, as clustering based on monthly values for each parameter would result in an overly large number of attributes to cluster. The average annual capacity factor, and the variation of the monthly capacity factors from the average annual value, was determined based on the provincial values calculated previously, and the average deviation for a given month and technology was calculated considering all the provinces. These average deviation values were then used to calculate monthly capacity factors for each cluster from the average annual value.

2) Energy System 2050 Parameters and Constraints : The maximum shares of public mobility and freight train mobility are maintained at 0.3 and 0.8 per cluster, respectively. In this case, the maximum DHN share is assumed to be proportional to the percentage of urban area of each cluster,

As before, a constraint regarding the maximum grid penetration of VREs is implemented. However, in this case the constraint is imposed over the entire system, rather than at the level of a single cluster:

$$\sum_{c}\sum_{t}(F_{t(PV,t,c)} + F_{t(Wind,t,c)}) \cdot t_{op(t)} \leq 0.7 \cdot \sum_{c}\sum_{t}\sum_{m} F_{t(m,t,c)} \cdot t_{op(t)} \cdot layers_{in,out(n,elec_{grid})} \quad (21)$$

IV. Model Validation

In order to verify the validity of the model, the adapted ES Canada model was used to model a reference energy system - in this case, the energy system of Canada in 2018 - with known parameters. Comparing the model output with the known parameters of the energy system allows for validation of the model. Tables VIII and VIII show the results of the model validation.

The values of the model objectives - total cost and GWP - for the cost minimized system - are also shown in Table VII. Canada emitted a total of 728 Mt CO_2^{eq} in 2018 [44], with 336 Mt CO_2^{eq} from the transport, buildings and electricity sectors. The remaining emissions are divided between the oil and gas sector (191.4 Mt), and waste and others (51.3 Mt) - which are not accounted for in ES - as well as heavy industry (77.1 Mt) and agriculture (73.1 Mt), of which only the emissions due to energy consumption are accounted in the model, while other emissions - such as the emissions due to cement production or animal manure - are not considered. Therefore, the model result seems to be within the range expected based on the actual system.

TABLE VII
2018 Reference System - MILP Model Objectives (Minimized Total Cost)

Total Cost	[BCAD/year]	700
Total GWP	[MtCO_2^{eq}/year]	344

TABLE VIII
Model Validation for 2018 Reference System - Resource Use

Resource	**MILP Model** TWh	**Actual** TWh	**Delta** TWh	**Delta** %
Coal	126	176	50	0.28
NG	1193	1233	39	0.03
Diesel	327	354	26	0.07
Gasoline	437	424	-14	-0.03
LFO	123	144	21	0.15
Uranium	245	249	3	0.01
Wood	161	133	-28	-0.21

TABLE IX
Model Validation for 2018 Reference System - Electricity Generation

Resource	**MILP Model** TWh	**Actual** TWh	**Delta** TWh	**Delta** %
Uranium	91	95	4	0.04
Hydro	364	382	18	0.05
Solar	2.9	3.1	0.2	0.05
Wind	30	32	2	0.05
Coal	44	53	8	0.16
NG	47	66	19	0.29
Petroleum	2	4	2	0.56
Biomass	2	9	6	0.74
Total	584	644	60	0.09

It can be seen from the validation results that the ES model is able to represent quite closely the reference system, with a percent difference between the model output and the actual system of less than 10% in many cases when considering total resource use as well as electricity generation.

This being said, there remain some cases for which the percent difference is greater - in particular, the total use of coal, LFO and wood, as well as the electricity generated by coal, gas, petroleum and biomass.

These differences can be explained as follows. First, the lower value of electricity generation by gas, petroleum and biomass determined by the model as compared to the actual system - and the lower overall electricity generation - can be attributed to an assumption made when defining the end use demands. As discussed in section III-A1, for industrial energy demand it was assumed that the electricity demand was only the direct electricity consumption by industry, and the demand fulfilled by other resources was attributed to heating. In reality, it is likely that a percentage of resource use - in particular, a percentage of the use of coal, NG, petroleum and biomass - was used for electricity generation rather than heating. Thus, it is likely that the electricity demand is slightly underestimated and the heating demand slightly overestimated in the model. However, as additional data regarding the percentage of demand attributed to electricity versus heating was not available, the original assumption was maintained.

The differences in overall resource use may be explained by differences in the efficiencies of technologies used by the actual energy system, and those energy scope model. For example, the efficiency of coal power plants in ES are 0.49 and 0.54 for US and IGCC plants respectively. However, these are relatively modern and efficient coal electricity generation plants, and many existing plants likely have a lower efficiency, thus resulting in a higher primary energy consumption in order to fulfill the same end use demand.

Further, it is important to recall that the model output is based on optimization of the total cost of the energy system, whereas the actual system has evolved in a way that is not necessarily optimal. Therefore, the model may present a configuration that uses more or less of a certain resource or technology in order to optimize the costs of the system. Although constraints were added in order to force to some extent the use of certain resources and technologies and mitigate this effect, some degree of flexibility was maintained, and this can also explain some of the differences observed between the model output and the actual system.

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