



OESM-IE: Open Energy System Modelling for Ireland

SEAI Research Award: RDD246

Technical Report WP3-D2

SWIS-100-IE Open Energy System Model for Ireland: 100% Zero-Emission Sources with CO₂ Removal (CDR)

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Executive Summary

This is the final technical report for the OESM-IE research project³. This project has been funded by the Government of Ireland through the Sustainable Energy Authority of Ireland under the SEAI National Energy Research, Development & Demonstration Funding Programme 2018, grant number 18/RDD/246. It was designed to support technical and economic modelling of potential future configurations of the Irish energy system that are dominated (up to 100%) by variable renewable primary sources (wind and solar), coupled with very large scale heterogeneous energy storage to facilitate interseasonal energy-time arbitrage. The scope encompasses all major energy final use sectors: direct electricity, heating and transport (including aviation). It provides for integrated production, storage, and diverse use of gaseous and liquid (including hydrocarbon) synthetic fuels, as well as net removal of carbon dioxide from atmosphere and transfer to secure geological storage. Further, for reproducibility, transparency, and to support future work, the project was undertaken with an explicit commitment to release of all models, tools and datasets under the most permissive feasible open development licensing. The project provides new tools to explore policy options and path dependencies likely to directly impact on Irish energy system development within the next two to three decades. It particularly addresses the context of limiting further national cumulative carbon dioxide emissions within the now very stringent limits of a national "fair share" of the finite remaining global cumulative carbon dioxide "budget" that is consistent with the temperature goals of the Paris Agreement.

This report is the formal deliverable of project Work Package WP3. It details the design and general use of the SWIS-100-IE Open Energy System Model for Ireland. This is the culmination of the technical development carried out in the project. SWIS-100-IE allows the exploration of potential energy system scenarios based exclusively on the use of *unequivocally* zero-CO₂ primary energy sources (wind, solar and nuclear). It is characterised as *functionally and spatially coarse grained* but *temporally fine grained*. This facilitates tractable exploration of the large scale space of strategic approaches to Irish energy decarbonisation, while still reflecting the multi-scale temporal constraints of matching overall primary supply from time-varying sources with time-varying demands, mediated via heterogeneous energy storage systems. Overall energy balance is required, but detailed levels of infrastructure deployment and energy flow dispatch are resolved by myopic optimisation of notional costs (with a time envelope of approximately 1-5 years). The model integrates datasets of historical energy demand, key weather related variables (high time resolution capacity factors for variable renewable electricity generation, and air temperature driving low temperature heat demand), and heat pump performance.

The body of the report details the internal architecture of SWIS-100-IE; provides guidelines for installation and execution of the model; and gives a series of illustrative examples of its use. It also outlines specific directions for planned future work, both applying the model and developing it further. The final concluding section summarises the specific respects in which this work has demonstrated significant novelty and represents advances beyond the pre-existing state of the art.

³https://sites.google.com/a/dcu.ie/dcuecrn/projects/oesm-ie

Table of Contents

1. Introduction	1
2. SWIS-100-IE: Open Energy Model	4
2.1 Architecture Overview	4
2.2 Detailed Subsystem Decomposition	8
2.2.1 Core Electricity and Energy Storage Subsystem	8
2.2.2 Carbon Dioxide Removal (CDR) subsystem	10
2.2.3 Low temperature heat subsystem	11
2.2.4 Surface transport subsystem	12
2.2.5 Air transport subsystem	14
2.3 Technology database	16
2.4 Installation	17
2.4.1 Cloud-based use	17
2.4.2 Local use	19
2.5 Execution	20
2.5.1 Single run jupyter notebook	20
2.5.2 Batch run jupyter notebook	21
2.5.3 Batch run command line script	22
3. Illustrative SWIS-100-IE Runs	23
3.1 Single run examples	23
3.1.1 Core Electricity and Energy Storage Subsystem	24
3.1.2 Addition of Carbon Dioxide Removal (CDR) subsystem	26
3.1.3 Addition of low temperature heat subsystem	29
3.1.4 Addition of surface transport subsystem	33
3.1.5 Addition of air transport subsystem: full system functionality	35
3.2 Batch run examples	38
3.2.1 Varying time resolution	38
3.2.2 Varying weather year	41
4. Future Work	45
5. Conclusion: Innovation/Novelty – Beyond State-of-the-Art	47
6. References	49
Appendices	51
A.1 Project RDD246: Original WP3 Summary	51
A.2 Software and datasets: Open Release	52
A.3 SWIS-100-IE configuration parameters	53

1. Introduction

Under the stringent requirements implied by the Paris Agreement temperature goals (UNFCCC 2015), and its commitments to international equity, nett CO₂ emissions in developed, industrialised, economies (such as Ireland's) will need to fall to zero, and then go negative (nett removal), much faster that current policies suggest — likely within two decades or less (McMullin et al. 2019; McMullin and Price 2020; McMullin 2020). Existing research suggests that the most technically feasible and cost-effective approaches will require a combination of demand constraint and integration of all energy demand sectors and energy carriers. This will likely involve aggressive deployment of zero-emissions variable renewable electricity generation (VRE: wind, solar, etc.), significant electrification of heating and transport, and deployment of some dedicated energy storage *within* the electricity sector (battery, pumped hydro, CAES); but it is unlikely that it can feasibly rely on universal electrification of all energy use. Rather, there will also be a significant need for heterogeneous *large scale energy storage*: including integrated production, storage, and diverse use of gaseous and liquid (hydrocarbon) synthetic fuels. The latter will require managed cycling of carbon dioxide (CO₂), via capture at the point of production if feasible but otherwise relying on air capture.

The OESM-IE project⁴ (SEAI reference RDD246, February 2019 - March 2021) was designed to support technical and economic modelling of such explicitly negative-CO₂ energy system scenarios for Ireland. Further, for reproducibility, transparency, and to support future work, the project was undertaken with an explicit commitment to release of all models, tools and datasets under the most permissive feasible open development licensing (Robbie Morrison and et al 2017; Pfenninger et al. 2018). The project provides early insight into policy options and path dependencies likely to directly impact on Irish energy system development within the next two to three decades.

This technical report details the design and general use of the SWIS-100-IE Open Energy System Model for Ireland⁵, developed and released under Work Package WP3 of the OESM-IE project. SWIS-100-IE is the culmination of the technical development carried out in the project. It is a software package, developed in python, and built on the PyPSA (Python for Power Systems Analysis) framework (Tom Brown and David Schlachtberger 2018)⁶.

SWIS-100-IE allows the exploration of potential energy system configurations for Ireland, based exclusively on the use of *unequivocally* zero-CO₂ energy sources (wind, solar and nuclear), with the additional option of requiring *removal* of CO₂ from atmosphere to secure, long term, storage (CDR). It is characterised as *functionally and spatially coarse grained* but *temporally fine grained*. That is, the model is deliberately designed to offer only a simplified, schematic, set of system configuration options. All major elements are spatially aggregated at a national level (demand sectors, energy sources, storage and conversion systems). This facilitates tractable (even interactive) exploration of the large scale space of strategic approaches to Ireland's future energy system, including the ability to investigate the general structure of interactions between the major functional choices. However: it is temporally fine grained (potentially down to one hour time resolution over periods of up to five years). This fine temporal resolution is essential to meaningfully represent the interactions in time between varying energy sources, energy demands and energy storage. Without this high time resolution, it is impossible to assess the specific needs and scale of energy storage potentially required in such systems. SWIS-100-IE is thus complementary to modelling approaches which

⁴https://sites.google.com/a/dcu.ie/dcuecrn/projects/oesm-ie

⁵https://github.com/bmcmullin/SWIS-100-IE

⁶https://PyPsa.org/

focus instead on much finer grained functional and spatial representations such as, for example, the IEA-ESTAP **TIMES** family of models (Loulou et al. 2005), including the Ireland-specific **Irish-TIMES** (Ó Gallachóir et al. 2020), or **EnergyPlan** (Lund 2017).

The SWIS-100-IE model integrates a suite of historical demand datasets, covering conventional electricity use, low temperature (space and water) heating, and transport (surface and air). It also incorporates historical datasets for key weather related variables: high time resolution capacity factors for solar PV and wind (onshore and offshore) electricity generation, and heat pump coefficient of performance (reflecting air temperature).

SWIS-100-IE is a so-called "capacity expansion" model: for a given run, it uses an externally provided Linear Programming solver to automatically identify the notionally optimal sizes of all major infrastructural elements in order to meet the specified sectoral demand profiles over the full period of any given run on a basis of least notional cost. The *dispatch* of the deployed infrastructural capacities is also simultaneously optimised across all time intervals ("snapshots") making up the run. For background theory of Linear Programming based optimisation see, for example (Vanderbei 2020). Optimisation is contingent on an included database of notional capital cost estimates (and other relevant technical parameters) for each associated technology. It must be emphasised that these *are* only estimates: and past experience of energy system technology development indicates that actual deployment costs can change very dramatically over time, diverging substantially even from expert projections (e.g., Hoekstra 2018; Evans 2020). The notional cost optimisation is described as *myopic*: that is, it is exclusively governed by the circumstances (demand and weather profiles) specified on a given run — typically of one to five year duration.⁷ Capital costs are amortised over the expected lifetimes of the distinct capital assets.

The use of linear optimisation based on (notional) costs means that the model also automatically yields so-called *shadow price* information associated with the various energy flows in any given run. Informally, these correspond to the prices that idealised markets would clear at (at each point where energy flows would be traded) to exactly cover all the notional costs attributable to the deployment and operation of the system. These can yield useful insights into the relative costs attaching to energy flows both in time and in different forms. However, *such reported shadow prices should be interpreted with considerable caution*. They rely both on the underlying, uncertain, notional cost estimates, and on the assumptions of perfect market operation. Further, depending on the exact model structure, even idealised markets can deliver so called "windfall" profits to certain elements of the system considered in isolation; which might, or might not, be redistributed in real world system deployment (through taxes and subsidies etc.) which would further perturb the prices actually prevailing.

Any single SWIS-100-IE solution effectively describes a "steady state" energy system configuration optimised relative to the specific demand and weather profile over the modelled period. The optimisation is premised on perfect foresight over the full run period, which would not, of course, be the case in real system operation. Further, such optimisation neglects real-world needs for contingency or reserve capacity. There may potentially be many optimal or near-optimal solutions for any given run: thus it is generally important to explore the sensitivity of outputs to perturbation of parameters before drawing strong conclusions. SWIS-100-IE is neither designed nor intended to attempt notional cost optimisation over the longer, multi-decadal, time period that would be required, for example, to transition from the current energy system to some target, fully decarbonised system. Indeed, given the very large uncertainties already mentioned in long term cost estimates, it is at

⁷The absolute maximum period that can be covered by a run is a complex function of the temporal resolution, the performance of the configured linear optimisation solver, and the available computational resources. However, it is unlikely to perform satisfactorily for modelling periods much in excess of five years.

least questionable whether notional cost optimisation is a useful or appropriate tool over such extended periods (Trutnevyte 2016). More generally, in assessing preferences among real world energy system deployment or transformation scenarios, there are many critically important socio-political factors that cannot be readily or meaningfully represented in the form of notional costs, and therefore cannot be reflected by notional cost optimisation.

In keeping with the overarching commitment to open development underpinning the OESM-IE project, SWIS-100-IE has been developed using only tools and datasets that, as far as possible, are available under permissive open licencing. SWIS-100-IE itself has been released⁸ under the GNU General Public License Version 3⁹.

The rest of this report is structured as follows:

- Section 2 details the internal architecture and design of SWIS-100-IE, and outlines how to install and execute model runs.
- Section 3 presents, in summary form, a series of illustrative model runs using SWIS-100-IE. These demonstrate the wide scope for coarse-grained exploration of future Irish energy system configurations that is enabled using this tool.
- Section 4 outlines a programme of further research that is planned, based on the use, and further development, of SWIS-100-IE, but which goes beyond the remaining feasible scope of the OESM-IE project.
- Section 5 concludes with a discussion of the specific novelty and innovation of the work presented, and the ways in which is represents an advance on the pre-existing state of the art.

Finally, a selection of more detailed technical information is provided as appendix material.

⁸https://github.com/bmcmullin/SWIS-100-IE

⁹https://www.gnu.org/licenses/gpl-3.0.en.html

2. SWIS-100-IE: Open Energy Model

This section provides an overview of the SWIS-100-IE architecture, more detailed descriptions of each of the component sub-systems, a summary of the technology parameter database, and instructions for installing and executing the model.

2.1 Architecture Overview

The complete SWIS-100-IE architecture, as implemented in PyPSA, is represented graphically in Figure 1. Flows of distinct energy carriers are indicated by different coloured arrows as per the key in Figure 2. Note that flows may be unidirectional or bidirectional as denoted by the arrows. Carbon dioxide (CO₂) is modelled as a *pseudo* energy carrier, with (conserved) quantities potentially flowing between distinct stores or the carbon being incorporated into synthetic hydrocarbon fuel. Distinct PyPSA components are indicated by different graphical elements as per the key in Figure 3. Where all flows associated with a given component are of the same energy carrier, the component is colour coded according to the same colour key as shown for flows in Figure 2. Where a component is associated with flows of more than one carrier type (i.e. it represents a *conversion* between carrier types), it is coloured grey. In the PyPSA framework, only Link components are capable of such carrier transformations.

The SWIS-100-IE model consists of:

- Inelastic final end-use energy demands across four coarse-grained sectors: general purpose electricity use, heating (low temperature only), surface transport and air transport. These are each represented by a single, aggregated, PyPSA Load component. Each can be configured with either a fixed, constant, demand, or a time-varying demand based on a public dataset for some historical period. This is of high temporal resolution (down to 1 hour) for electricity and heating, but only low temporal resolution (annual) for transport. For historical demands, different base years may be chosen separately for each sector. Note that the available historical dataset years vary by sector. In the case of general purpose electricity demand, datasets can also be configured by political jurisdiction (Ireland or Northern Ireland) or on a combined, all-island, basis. For other final energy sectors, datasets are currently included only for Ireland.
- A coarse grained set of potential primary energy sources: wind (onshore and offshore), solar PV, and nuclear fission. These are each represented by a single, aggregated, PyPSA Generator component. Variable renewable energy sources (VRE: wind, solar) are scaled by high time resolution availability factors, based on public weather datasets for some historical period. While SWIS-100-IE is primarily focussed on modelling energy systems dominated by VRE sources, nuclear energy (premised on availability of suitable small modular reactors/SMR) is included as an additional, hypothetical fully dispatchable and "zero CO₂" (operational, not embodied) energy source. It should be noted that nuclear energy deployment within Ireland is currently prohibited on a statutory basis. Further, there are no indigenous sources of nuclear fuel, nor any existing reprocessing or waste disposal facilities. Each coarse-grained source can be configured with minimum and/or maximum allowed deployed capacity. Within these limits, the model will apply myopic optimisation of notional cost to fix a specific deployed capacity of each source, sufficient to meet the configured final energy demand over the (myopic) run period, in conjunction with all required configuration of conversion and/or storage components.
- One secondary energy source: environmental heat. This is shown with a dotted outline (denoted "Heat RE") in Figure 1. This reflects the fact that this source is only *tacitly* represented in the underlying PyPSA model. It is properly classified as a *secondary* energy source because

its availability is contingent on the supply of energy (electricity) from some upstream (primary) source. It is implemented in SWIS-100-IE as a coupled effect of the deployment of the ASHP (aggregated air source heat pumps) Link component. Though this source is represented in the system diagram, it does not have a separate, explicit presence as a PyPSA Generator component.

- A coarse grained set of potential energy conversion processes, represented by PyPSA Link components. This also includes CO₂ transport and conversion processes, where CO₂ is represented as a pseudo-energy-carrier. Where appropriate these Links may also be configured with upper or lower limits on allowed power flow capacities. Within such limits, PyPSA again applies myopic optimisation of notional cost to fix a specific deployed capacity sufficient to ensure that the overall system final energy demands are met.
- Multiple PyPSA Bus components, as required, to integrate converging and diverging flows of a given energy carrier. Buses impose an analogue of the Kirchoff current law: all flows to and from any given Bus must balance to zero at all times. The core electricity and hydrogen buses can be interpreted as coarse grained representations of the national electricity grid and (putative) hydrogen gas pipeline network, respectively.
- Multiple, heterogeneous, coarse grained, material storage systems represented by PyPSA Store components. These are generally for storing *real* energy carriers (electricity directly in batteries, hydrogen, synthetic hydrocarbon fuel/synfuel), but are also used to represent storage of the *pseudo*-energy-carrier, CO₂.
- International electricity interconnection, also represented in a coarse grained manner by a PyPSA Store component. This may be configured with a finite maximum energy capacity to represent a limit to cumulative imbalance between import and export at any time within a run.

Note that *all* stores of real energy are constrained to balance over a complete run: that is, all energy demand must be met directly or indirectly by the energy sources *within* the system over the run. There can be no net import or export over interconnection, nor net drawdown of internal energy stores.

There are two non-energy, or *pseudo-energy*, stores, associated with the pseudo-energy-carrier, CO_2 . One represents dilute CO_2 in atmosphere (to track net CO_2 transfer to or from atmosphere) and one represents concentrated CO_2 in some technological store (e.g., geological, such as a disused fossil gas field). A run may be configured to require a specified level of cumulative net CO_2 removal from atmosphere ("net negative" emissions) over its course. This would necessarily correspond to an exactly equal net cumulative *increase* in the store of concentrated CO_2 over the run.



Figure 1: SWIS-100-IE Overall system architecture



Figure 2: SWIS-100-IE energy carrier colour key



Figure 3: SWIS-100-IE PyPsa component icon key

2.2 Detailed Subsystem Decomposition

To understand the detailed design and operation of the SWIS-100-IE model, it is helpful to decompose the system as a whole into a small number of loosely coupled *subsystems*.

In the subsystem diagrams that follow, flows *between* subsystems are tacitly represented by the presence of common buses.





Figure 4: SWIS-100-IE Core electricity and storage subsystem

The SWIS-100-IE core electricity and energy storage subsystem is shown in Figure 4. This constitutes the *core* of SWIS-100-IE in the sense that it can function as a free-standing system that can fully service the general electricity end use Load (local-elec-demand); while each of the other subsystems *requires* this core system as a basis, but successively adds the capability to service some discrete, additional, category of energy service demand.

The direct outputs of all the primary energy sources in SWIS-100-IE are in the form of electricity, and these are all included in the core subsystem. None of the other subsystems add additional primary energy sources: thus, *all* final energy needs must ultimately be served by deployment of sufficient primary energy supply within the core subsystem.

Technology and cost parameters for nuclear-SMR are drawn from (18-for-0 2020). High time resolution normalised historical variability data of wind (onshore and offshore) and solar generation, expressed as estimated nominal capacity factor (in the absence of dispatch down), specific to Irish

geographical territories, are drawn from the renewable.ninja¹⁰ open datasets; see (Pfenninger and Staffell 2016) and (Staffell and Pfenninger 2016) for the detailed methodologies and validation processes underlying these. High time resolution historical direct electricity load data is derived from datasets made available by the Eirgrid, the Irish Transmission System Operator¹¹; unfortunately no explicit open licencing information is associated with these.

Given that the nuclear-SMR Generator is fully dispatchable, if it is allowed to be deployed with arbitrary capacity, then the core subsystem *could* successfully solve (meet an arbitrary electricity Load profile) even without any energy storage capability. However, in the intended application of SWIS-100-IE, the VRE sources (solar, onshore wind and offshore wind) are expected to dominate supply: i.e., nuclear-SMR will typically be either disallowed, or constrained to a relatively limited maximum power capacity.

Given large scale (inter-seasonal) temporal mismatch between VRE availability and the inelastic load, and recognising that arbitrarily large VRE over-provisioning (with correspondingly large curtailment/arbitrarily low capacity factor) would be neither technically or economically feasible, it is essential to include energy-time shifting (arbitrage) functionality even in this core subsystem. To allow investigation across a representative range of possible support technologies, three heterogeneous forms of energy-time shifting are implemented, corresponding to: hydrogen storage, battery storage, and time arbitrage of energy over international electricity interconnection. Each of these allows potential for flexible temporal shifting of energy to balance the instantaneous flows between sources and the (inelastic) Load. Each option has different characteristics in terms of losses and costs, and each may also be subject to specific constraints on the deployable capacities (power and/or energy).

Hydrogen storage comprises a H₂ Store, together with a H₂ electrolysis Link to convert from electricity to hydrogen and two possible generation pathways from H₂ back to electricity, namely combined cycle gas turbine (CCGT) or open cycle gas turbine (CCGT). The power capacities for electrolysis, CCGT and OCGT can all be independently optimised. Note that within this core subsystem there is no direct (final) use of hydrogen energy: it functions solely as an intermediate carrier for storage purposes. Battery storage, involving no change of energy carrier, is represented by a Store component and separate charge and discharge links. However, as these links effectively correspond to the same (bi-directional) hardware, the charge and discharge power capacities are constrained to be equal. International electricity interconnection is modelled in a coarse grained way as structurally similar to battery storage (no change of energy carrier, formally separate IC-import and IC-export Links, again constrained to have the same power capacity), but, of course, with different underlying cost parameters.

Note that the PyPSA framework offers an alternative StorageUnit component which combines the energy store with the charge and discharge functionality. However, that does not allow separate optimisation of the power and energy capacities (it relies on a fixed scaling between power capacity and energy capacity expressed in full-power discharge hours). In SWIS-100-IE it was preferred to allow independent optimisation of power and energy capacities, hence the decomposition into Store components and suitably constrained Link(s) components for charge/discharge.

It is important to emphasise again the *functionally coarse-grained* nature of SWIS-100-IE. In the case of the core electricity subsystem, he model scope does not address the spatial characteristics of transmission or distribution: so *network constraint* on power flows (as opposed to *system-wide curtailment*) is not represented: it is effectively assumed that (in steady state) sufficient network

¹⁰https://www.renewables.ninja/

¹¹http://www.eirgridgroup.com/how-the-grid-works/renewables/ (under System and Renewable Data)

capacity will be deployed to avoid significant constraint. Similarly, issues such as system stability (inertia, reserves, individual unit commitment and ramp rates etc.) are not represented. In relation to synchronous non-synchronous penetration ratio (SNSP) in particular, it is assumed that technical measures can be identified to allow running at 100% instantaneous supply from VRE sources (whether through deployment of synchronous condensers, synthetic inertia or other means).





Figure 5: SWIS-100-IE Carbon Dioxide Removal (CDR) sub-system

Figure 5 shows the SWIS-100-IE Carbon Dioxide Removal (CDR) subsystem. This adds support to impose a constraint for *net removal* of CO₂ from atmosphere and transfer to a non-atmospheric store. This is achieved through the deployment of so-called direct air capture (DAC) technology, and the provision of sufficient additional energy supply to achieve the required level of net removal over the run (but with full flexibility on timing within the run). This is a coarse and schematic representation of possible routes to CDR. It deliberately eschews biogenic removal (for example via bioenergy combined with carbon capture and storage, or BECCS). This is based both on the extremely poor energy efficiency of biogenic energy capture (compared even to solar PV) and on the conservative assumption that large scale BECCS (especially based on internationally traded bioenergy fuels) would present severe risks of food insecurity, increased deforestation, and biodiversity loss. Further, although currently envisaged DAC technologies typically require the greater part of the energy input to be in the form of relatively high temperature heat, the implementation here assumes all energy input to be in the form of electricity. This is based on the fact that all the available primary energy sources in this system yield electricity anyway, so there is unlikely to be any material saving by configuring the DAC system with multiple distinct input energy carriers. Thus any required conversion (from electricity to heat) is tacitly internal to the DAC Link. It should be emphasised that DAC technology has only been deployed at pilot scale to date (Keith et al. 2018; IEA 2020), remains at a low technology readiness level, and notional cost estimates are

therefore especially uncertain for this subsystem.

The CDR system is contingent on the deployment of the SWIS-100-IE core. If it is required purely for *removal* of CO_2 from atmosphere into "permanent" storage (secure for multi-century timescales) then it is independent of the presence of other subsystems. However, it can also be deployed to provide a source of CO_2 for *utilisation* if that is required. In the current SWIS-100-IE architecture, this potentially arises for one other subsystem, namely air transport, where CO_2 is required as an input for the production of synthetic liquid (hydrocarbon) fuel.



2.2.3 Low temperature heat subsystem

Figure 6: SWIS-100-IE Low temperature heat subsystem

Figure 6 shows the SWIS-100-IE low temperature heat subsystem. Low temperature (space and water heating) is characteristically seasonal in Ireland. In order to effectively model the interactions between such heat energy demand patterns and seasonally variable renewable energy sources, with a consequent potential role for interseasonal energy storage, it is essential to represent this heat demand with high temporal resolution (ideally down to 1 hour). No *instrumental* datasets of low temperature heat demand, with such high time resolution, have been identified for Ireland (under open licencing or otherwise). However, an open *synthetic* dataset of low temperature heat demand was identified via the when2heat project¹². As detailed by (Ruhnau et al. 2019) this uses open data on population, building types and historical weather to synthesise high time resolution historical demand profiles, aggregated at national level, for 16 European countries, including Ireland. This is incorporated into the lo-temp-head-demand Load in SWIS-100-IE. The historical start year and period can be arbitrarily configured (within the available dataset) for any given run.

Two possible, coarse grained, pathways for meeting this demand are made available, drawing on primary energy supply from the core subsystem: either direct combustion of hydrogen (in high efficiency condensing boilers) or via (air source) heat pumps driven by primary electricity but then harvesting secondary energy from environmental heat.

A further advantage of the when2heat dataset is that it also includes synthesised, high time resolution, estimates of coefficients of performance (CoP) for both air- and ground-source heat pumps, servicing either space or water heating. In the implementation in SWIS-100-IE, this is used

¹²<u>https://data.open-power-system-data.org/when2heat/</u>

to configure the behaviour of the single aggregated air source heat pump Link component (denoted ASHP).

Maximum power capacities for the ASHP and H2 boiler pathways can be configured. Within the allowed ranges, PyPSA will then apply myopic optimisation of notional cost to fix a specific deployed capacity of each in any given run.

Note that the aggregation and coarse graining in this subsystem does represent a significant simplification in that it tacitly allows the Load in any time interval to be met by an *arbitrary* combination of the available ASHP and H2 power capacities. This ignores the reality that both the Load and the ASHP and H2 boiler equipment would consist of many physically discrete, spatially distributed, installations, that do not support transport of produced *heat* from an arbitrary heat source to an arbitrary demand location. Nonetheless, even this coarse grained and schematic representation can still serve to provide a general indication of the relative scales of capacity that might be required of each pathway, and their patterns of use over time, even if only in highly aggregated form, as well as giving a good quantitative indication of the scale of upstream primary energy required to support servicing this overall demand.

Of course, in addition to low temperature heat, in the energy system as a whole, there is also a material requirement for high temperature heat, particularly in industrial processes. This is likely to be significantly less seasonal than low temperature demand; but no high time resolution datasets of industrial heat demand in Ireland have been identified in any case (whether instrumental or synthetic, under open licence or otherwise). The representation of high temperature (industrial) heat demand has therefore been omitted from the initial release of SWIS-100-IE; but it is planned for future incorporation, on the basis of reconciling the (synthetic) low temperature datasets with the separate, low time resolution (i.e., annual) SEAI data on *total* heat demand.



2.2.4 Surface transport subsystem

Figure 7: SWIS-100-IE surface transport subsystem

Figure 7 shows the SWIS-100-IE surface transport subsystem. This consists of a single PyPSA Load component, representing aggregate surface transport energy demand, and two possible conversion pathways whereby this demand may be met: using electricity via a fleet of battery electric vehicles (represented by the aggregate BEV Link) and/or using hydrogen via a fleet of hydrogen fuel cell electric vehicles (represented by the FCEV Link). In both cases, the required energy flows (electricity or hydrogen) would have to be provided from the core subsystem (via

appropriate additional deployment of one or more of the core primary energy sources).

As for high temperature heat, no high time resolution datasets of surface transport energy demand in Ireland have been identified. Nonetheless, surface transport is a very substantial component of overall energy demand in Ireland and has therefore been integrated into the initial SWIS-100-IE release, albeit in comparatively simplified form. In this case, the temporal demand profile is generated by upsampling of the low time resolution (annual) datasets provided by SEAI¹³, with linear interpolation between years. Note that, unfortunately no explicit open licencing information is associated with these SEAI datasets. Given that transport energy is currently almost entirely serviced by internal combustion engine (ICE) vehicles using fossil hydrocarbon fuels (petrol and diesel), the SEAI demand data is generally expressed in terms of such fuel quantities delivered to vehicle tanks, rather than the corresponding end-use (mechanical) energy. However, in the SWIS-100-IE context, given that the only vehicle options nominally deployed will be battery electric and/or hydrogen fuel cell, and given that both of these technologies offer much different (higher) tank-towheel (mechanical energy) conversion efficiency than ICE vehicles, the SEAI hydrocarbon fuel (tank) energy data is scaled to putative mechanical (wheel) end use energy demand. This allows SWIS-100-IE model runs to reflect the efficiency gains that arise from surface transport drivetrain electrification (whether via BEV or FCEV). A single aggregate ICE efficiency factor is applied for this purpose, nominally representative of the current ICE vehicle fleet. This is configured in the systemwide technology database (see section 2.3), along with notional fleet-wide conversion efficiency factors for the alternative BEV and FCEV pathways. But it remains important, when interpreting output data from SWIS-100-IE, to emphasise that the reported surface transport energy load is mechanical (wheel) based; and will therefore be systematically less that the reported "final" energy delivered to vehicle tanks in the original historical datasets. Nonetheless, the reported load will still correspond to full delivery of the identical historical surface transport services.

To support the notional cost optimisation of capacity expansion on SWIS-100-IE, it is necessary to specify notional capital cost (CAPEX) estimates (assumed to scale with power capacity) for each of the aggregated fleet types (BEV and FCEV). This is necessarily a somewhat arbitrary process. It properly depends on complex interactions between technology developments, manufacturing scale, underlying costs and user preferences across different vehicle models potentially making up such an aggregated fleet. The simple approach adopted in SWIS-100-IE is to take just one "representative" vehicle model as a basis for the fleet. But even with that simplification, to establish a scaling factor between CAPEX and fleet power capacity, one needs some estimate of the capacity *factor* or average utilisation of each vehicle. The method adopted for this is again very coarse grained. A notional average annual vehicle travel distance is assumed, with average energy consumption referenced to the selected representative vehicle model. This then allows relating a specific CAPEX to a specific (average) available power consumption, and this ratio is taken to be notionally representative of the full fleet. Further details of these calculations are documented in the system-wide technology database (section 2.3).

As was the case with the low temperature heat subsystem, aggregation and coarse graining in the surface transport subsystem does represent a significant simplification in that it tacitly allows the (mechanical) surface transport energy load in any time interval to be met by an *arbitrary* combination of the available BEV and FCEV power capacities. But these components actually each represent separate *fleets* of discrete, spatially distributed, vehicles; and of course, there is no actual mechanism that would allow an arbitrary transport *service* need in one spatial area (i.e., a discrete journey) to be met by an arbitrary vehicle (from either fleet), potentially located in an arbitrarily

¹³https://www.seai.ie/data-and-insights/seai-statistics/key-statistics/energy-data/ (under Energy Data as Timeseries | Energy Flows)

different spatial area. Even *within* the aggregated vehicle types (BEV and FCEV), and even supposing both types are spatially distributed, co-located with all particular demands, different vehicle categories (trucks, buses, cars etc.) within these general fleet types would still not be arbitrarily interchangeable with each other in servicing specific service demands. But notwithstanding these necessary limitations of the functional coarse graining approach, and again as for the low temperature heat subsystem, SWIS-100-IE can still serve to provide a general indication of the relative scales of overall capacity that might be appropriate to each fleet type (BEV and FCEV), as well as giving a good quantitative indication of the scale of upstream primary energy required to support servicing the overall surface transport demand.

SWIS-100-IE does not attempt to represent the breakdown of the surface transport fleet across vehicles of different capacities, nor the mapping of transport services (passenger-km or tonne-km of freight) onto such varying capacities. Thus, the model does not explicitly capture the potential for significant energy efficiency improvement through achieving higher shares of shared-mode occupancy for passenger transport, such as vehicle pooling, ride-sharing and conventional public transport. It is known that this potential is very substantial (e.g., Petrik and Martinez 2018); and that, on pure cost-optimisation criteria essentially all passenger transport would be switched to such modes (e.g., Oireachtas 2018, remarks by Prof. Brian O'Gallachóir). Given the limitations of notional cost-optimisation, it is considered sufficient that such possibilities can still be implicitly explored in SWIS-100-IE, in a functionally coarse-grained way, by prior rescaling of the final transport service demand (outside of the model) to reflect some estimated overall efficiency improvement due to increased vehicle occupancy and/or take up of alternative transport modes (Carroll 2018). More integrated support for demand rescaling is planned to be added to SWIS-100-IE in future work.



2.2.5 Air transport subsystem

Figure 8: SWIS-100-IE air transport subsystem

Figure 8 shows the SWIS-100-IE air transport subsystem. As with surface transport demand, no high time resolution datasets of air transport energy demand in Ireland have been identified. Nonetheless, air transport is another significant component of overall energy demand in Ireland and has therefore been integrated into the initial SWIS-100-IE release. The demand profile has been constructed with the same methodology as was used for surface transport, via upsampling of data

drawn from the same low time resolution (annual) fuel consumption datasets provided by SEAI, with linear interpolation between years. For consistency with the representation of surface transport data, air transport demand has also been coarsely rescaled to reflect end-use *mechanical* energy in flight, rather than raw fuel energy delivered to aircraft tanks (based on a notional average jet engine conversion efficiency).

However, the plausible strategies for servicing air transport demand with zero emissions remain much more constrained than for surface transport. While there is significant research on novel aircraft designs using zero emission fuels (electricity, hydrogen, ammonia), this remains early stage, with very severe technical obstacles to achieving performance (payload and range) at all comparable to the current global aircraft fleet (Murphy 2018). Together with the large sunk investment in this existing fleet, there is a strong basis for studying approaches that focus instead on "drop in" fuel replacement. That is, allowing continued use of liquid hydrocarbon fuels on board (existing and new) aircraft, with continued CO_2 release to atmosphere in flight; but with some mechanism to recycle this carbon back into fuel, as opposed to the current, one way, cumulative, transfer of carbon in *fossil* fuels from secure geological storage into atmosphere. There are then essentially only two distinct techniques, depending on whether the removal of CO₂ from atmosphere is biogenic (yielding liquid biofuels) or via technological means (DAC). Reliance on biogenic removal essentially means securing sufficient bioenergy production resource - land, water, etc. - to support this. As already discussed in relation to the carbon dioxide removal subsystem (CDR, section CCC), in the design of SWIS-100-IE it was decided to take the conservative position of eschewing reliance on very large scale expansion of bioenergy production on a global scale. This reflects the severe risks of food insecurity, increased deforestation, and biodiversity loss that such reliance may present. Instead, the air transport subsystem is built on the CDR subsystem, relying on the latter for supply of CO₂ removed from atmosphere. This is combined with hydrogen in a production pathway for synthetic hydrocarbon liquid fuels. This is nominally denoted as a Fischer-Tropsh process, but without prejudice to the development of alternative conversion processes that may be more appropriate than conventional Fischer-Tropsh with these particular feedstocks (Schmidt et al. 2018; Goldmann et al. 2018; He et al. 2019).

A synthetic fuel buffer store is included, configured with notionally zero CAPEX cost and zero efficiency losses. This reflects the fact that the costs of such liquid fuel storage are expected to be negligible compared to the other energy storage options in this model (specifically battery and hydrogen), and energy losses will also be comparatively very small. Thus it will make sense to avail of all potential time arbitrage of synthetic fuel production. This effectively decouples the timing of production and use of synthetic fuel. This is manifested in the shadow price of synthetic fuel being decoupled from time variations in upstream energy costs (electricity for DAC and/or hydrogen production), and instead being constant over the run period.

The (now conventional) aircraft fleet is represented by a single coarse grained aggregate Link, converting this synthetic fuel to end-use mechanical energy in flight. This is parameterised (CAPEX and fuel efficiency) on the basis of publicly available data for a single representative aircraft model, and public data on typical fleetwide aircraft capacity factor ("average daily airbourne hours"), as detailed in the system-wide technology database (section 2.3).

It is important to note that the climate effects of aviation are not limited to CO_2 . There are also additional non- CO_2 effects, including emission of nitrogen oxides, contrails, and aviation-induced cirrus clouds (Larsson et al. 2019). While these additional effects are subject to greater uncertainties than the strictly CO_2 effects, they are certainly non-trivial, and may add as much warming effect again as the CO_2 impact alone. Thus, while the design of the air transport subsystem in SWIS-100-IE ensures that it is net zero in terms of CO_2 only emissions (through strict carbon recycling), this is not sufficient in itself to ensure that the total climate impact of the air transport sector is neutral. This *can* be addressed, within the SWIS-100-IE architecture, by imposing a constraint for *additional net removal* of CO_2 from atmosphere in proportion to the configured air transport load. Given the uncertainties in the estimation of the non- CO_2 effect, this is not preconfigured, but simply left to user determination in any given model run where the air transport subsystem is being activated. A more integrated configuration mechanism may be considered for development in a future release.

Given that the air transport subsystem offers only a single pathway to meet the air transport demand profile, no configuration options are offered to limit the deployed power capacities of the corresponding Link components (the notional Fischer-Tropsch synthetic fuel plant and the aircraft fleet): they are simply left open to be selected on the basis of notional cost optimisation, as necessary to meet the demand. As with the other subsystems, the required primary energy to support the air transport subsystem must be provided by additional deployment of more capacity in the primary sources in the core subsystem. Further, there will be increased deployment of hydrogen electrolysis in the core subsystem and of DAC in the CDR subsystem as required to respectively provide the specific hydrogen and CO_2 feedstock flows for the synthetic fuel production.

2.3 Technology database

SWIS-100-IE relies on a technology database to provide notional parameter estimates for:

- capital costs (CAPEX) on an "overnight build" basis
- expected asset lifetime
- fixed annual operating and maintenance costs (FOM) as a percentage of CAPEX
- cost of finance (discount rate/interest rate)
- energy conversion efficiency

Default (fall-back) parameter values are provided where relevant, which are used if technologyspecific parameters are not defined.

The various cost parameters are processed by SWIS-100-IE to produce an integrated annual, amortized cost parameter for each relevant deployed technology component, which scales according to the deployed capacity (power or energy as applicable).

Parameters are included in the database for three notional deployment years: 2020, 2030 and 2050. This allows the incorporation of projected cost evolution into the future. Any single model run is configured to use the parameters for one specified deployment year.

The database is implemented in the form of a single file in the Open Document¹⁴ spreadsheet format (usually denoted with the file name extension: **.ods**). While this can be opened (and edited) with common proprietary spreadsheet application software, it is recommended to use the open-source, cross-platform, LibreOffice software suite¹⁵.

The technology database bundled in the initial SWIS-100-IE release is derived from a more limited database originally distributed with the PyPSA/WHOBS open model¹⁶ (dispatchable electricity generation based on VRE and large scale hydrogen energy storage). It has been substantially expanded to address the much wider technology portfolio included in SWIS-100-IE.

¹⁴https://www.libreoffice.org/discover/what-is-opendocument/

¹⁵https://www.libreoffice.org/

¹⁶https://github.com/PyPSA/WHOBS

2.4 Installation

The initial release of SWIS-100-IE is in the form of an open, publicly accessible, repository hosted on the **github** service¹⁷. SWIS-100-IE builds upon an extensive suite of additional open resources, both software and datasets. These prerequisite resources must all be available in order to execute model runs in SWIS-100-IE.

There are two approaches to making this possible. One is to install all required prerequisites locally. While potentially complex, this is generally a one-time process and provides an environment that is then available for extended ongoing experiments using SWIS-100-IE; including, if desired, modification or customisation of the underlying implementation (i.e., potentially going beyond the provided configuration options). Alternatively, it is also possible to run SWIS-100-IE models using a cloud-based service. This *automates* the creation of a full execution environment, containing all required prerequisites, on a virtual cloud-based server. However, the created cloud-execution environment is not persistent: all runs must be completed (and results downloaded) within a time-limited execution session. Accordingly this is most suitable for users who wish only to use SWIS-100-IE for occasional experiments, and without any intention or requirement to modify the underlying implementation.

It should also be noted that the physical energy requirement to execute each cloud-based session may be comparatively high, precisely because of the overhead of dynamically creating the full execution environment on demand. So for users who do intend to undertake a significant number of runs, then creating a persistent, local, execution environment is likely to be significantly less demanding of physical energy.

Both approaches are described in more detail in the following sections.

2.4.1 Cloud-based use

Cloud based use of SWIS-100-IE is supported via the open **mybinder** service. This section summarises briefly how to access this service. A more detailed video screencast has also been released showing a full demonstration¹⁸.

The **mybinder** service is accessed entirely from within a web browser, without requiring any local installation of software or datasets. Any available **mybinder** application can be requested via a generic form (see Figure 9) at the **mybinder** home page URL:

https://mybinder.org/

To specify SWIS-100-IE manually in this form, proceed as follows:

- For gitHub repository name enter: bmcmullin/SWIS-100-IE
- For Git ref (version identifier) enter: master
- Finally, select: Launch

Alternatively, this initial dialogue form can be bypassed by directly visiting an application-specific target URL for SWIS-100-IE (which will also trigger automatic launching):

https://mybinder.org/v2/gh/bmcmullin/SWIS-100-IE/master

In either case, once launched, **mybinder** will check for a prebuilt (cached) image of the full SWIS-100-IE execution environment (dependent on whether other users have recently requested access to this). If such a prebuilt environment image is not available, then it will be built, but this may take

¹⁷https://github.com/bmcmullin/SWIS-100-IE/tree/master

¹⁸https://youtu.be/0TA-JSGoZmk

some time (perhaps 10 minutes or more). Once the built environment image is available, it will be queued ("pushed") for access to an execution server. Depending on overall demand on the service, this may also cause some further delay (indicated with the repeated message "Pushing image"). Once an execution server is available, the environment will be loaded, and an execution service started, represented by the appearance in the browser of a standard jupyter notebook service interface (Figure 10).

GitHub 🗸	bmcmullin/SWIS-100-IE			
Git ref (bran	ch, tag, or commit)	Path to a notebook file (optional)		
master		Path to a notebook file (optional)	File 🗸	

Figure 9: mybinder launch form (in web browser)

📁 Jupyter	Visit repo	Copy Binder link	Quit
Files Running Clusters			
Select items to perform actions on them.		Upload	New - 2
	Name 🕹	Last Modified	File size
Cassumptions	1	5 minutes ago	
batch-run-example	1	5 minutes ago	
D binder	1	15 minutes ago	
C doc	1	5 minutes ago	
		8 minutes ago	
	1	5 minutes ago	
		8 minutes ago	
	1	15 minutes ago	
		8 minutes ago	
C when2heat		8 minutes ago	
🗌 🧧 matplotlib-test.ipynb	1	5 minutes ago	826 B
🗌 🧧 SWIS-100-batch-run.ipynb	1	5 minutes ago	3.48 kB
🗌 🖉 SWIS-100-single-run.ipynb	1	15 minutes ago	33.8 kB
	1	5 minutes ago	35.1 kB
README.md	1	5 minutes ago	4.88 kB
Swis100.py	1	5 minutes ago	72.9 kB
Swis100_batch.py	1	5 minutes ago	2.02 kB

Figure 10: mybinder jupyter notebook interface (in web browser)

From this point, SWIS-100-IE may be used via either a single-run or batch-run **jupyter notebook** interface as detailed in sections 2.5.1 and 2.5.2 below. Note that *command line script* execution (section 2.5.3) is *not* possible using the **mybinder** cloud service.

As already noted, **mybinder** does not provide persistence of an execution image across sessions. Inactive sessions (with no ongoing execution and no user interaction) automatically terminate relatively quickly (approximately 10 minutes). It is therefore *strongly recommended* to download any results generated in a **mybinder** session as soon as they are complete.

2.4.2 Local use

Given the overarching commitment in the project to open tools and technologies, all development of SWIS-100-IE to date has been entirely on an (open) linux platform (using the mint distribution¹⁹). linux is the preferred or recommended platform, and is the only one on which the initial release has been systematically tested. Nonetheless, SWIS-100-IE itself, and the various additional packages and datasets on which it depends, is platform agnostic, and can be successfully deployed across all modelling platforms in common use, both open and proprietary (i.e., including linux, Microsoft Windows[™] and Apple macOS[™]). Cross-platform installation instructions are already available for the underlying PyPSA modelling framework²⁰. This includes installation of the conda²¹ software package manager, which itself provides a full python execution environment, and installation of a suitable, compatible, linear optimisation solver. The following steps are then required to install and run SWIS-100-IE specifically on the linux platform. Some platform-specific interventions will be required on other platforms, where indicated.

• Download a complete copy of SWIS-100-IE from the GitHub repository at:

https://github.com/bmcmullin/SWIS-100-IE/

- This may be downloaded either in the form of a single archive file (.zip archive format, which should be fully unpacked using the relevant local platform tools) or via the clone repository functionality of the open source git software revision control package²². The latter is preferred for users who may wish to contribute to the ongoing development of SWIS-100-IE. For users who wish only to *execute* model runs using the released system, then simple download and unpacking of the archive file is generally sufficient.
- Install any required remaining python packages via conda using the provided environment.yml file (in the binder subfolder). Under the linux command shell, this may be done as follows:

conda env create --name swis --file=binder/environment.yml

which will create a new conda environment (called swis) including the required packages. For all sessions using SWIS-100-IE, this environment should be *activated* as follows:

conda activate swis

These commands should be adapted as appropriate on other platforms.

¹⁹https://linuxmint.com/

²¹https://docs.conda.io/

²⁰https://PyPsa.readthedocs.io/en/latest/installation.html

²²https://git-scm.com/

• Download all required datasets. Under the linux command shell, this may be done automatically as follows:

binder/postBuild

This executes a linux command script. On other platforms, it will be necessary to examine the detailed commands in this script file (which can be opened with any local text editor) and manually carry out the required operations. This essentially involves downloading specified public dataset files and (in some cases) extracting specific required files from a container archive format.

Execution of SWIS-100-IE models, once the system is fully installed, is detailed in the next section.

2.5 Execution

SWIS-100-IE can be executed either interactively, within a web browser, using a jupyter notebook, or as a command line python script. Two notebooks are provided, one to configure and execute a single run with a variety of example interactive analyses and graphical plots, and one for executing a preconfigured batch of separate runs where the batch results can be saved to persistent files for subsequent post-processing. The command line script supports only the batch run approach. All three cases are explained in more detail in the following sections.

In the case of either of the notebook-based interfaces, the jupyter notebook server must first be started. Under the linux command shell, this can be done as follows:

jupyter notebook &

This will either open a new browser session (using the default web browser specified by the platform) or open a new tab in an already running browser session. This is then essentially identical to the interface provided when accessing SWIS-100-IE using the binder cloud-based service, as previously illustrated (Figure binder-jupyter).

From there, either the single-run or batch-run jupyter notebooks may be opened and executed, as detailed below.

2.5.1 Single run jupyter notebook

The single run jupyer notebook is called: SWIS-100-single-run.ipynb

It will open in a separate browser tab, with a standard jupyter notebook interface as illustrated in Figure 11.

Jupyter SWIS-100-single-run Last Checkpoint: 15/02/2021 (unsaved changes)	Logout
File Edit View Insert Cell Kernel Widgets Help	Trusted Python 3 O
🖺 🕂 🖗 🖓 🎝 🛧 V 🕨 Run 🔳 C 🕨 Markdown V 🖾 O git nbdiff	
SWIS-100 "Single Run" notebook	
Set up run (interactive/single-shot)	
In []: 1 import os 2 import numpy as np 3 import pandas as pd 4 import swis100 as swis	
<pre>In []: 1 display(swis.solar_pu_raw) 2 display(swis.wind_pu_raw) 3 display(swis.elec_load_data_raw) 4 display(swis.transport_load_data_raw) 5 display(swis.when2heat_data) 6 display(swis.assumptions_raw)</pre>	
<pre>In []: 1 run_config = {} run_config['solver_name'] = 'cbc' run_config['assumptions_year'] = 2030 # Used to select projected nominal technology costs # https://www.ecb.europa.eu/stats/policy_and_exchange_rates/euro_reference_exchange_rates/l # Change from 7 July 2019 to 8 July 2020 # Minimum (20 March 2020): 1.0707 - Maximum (9 March 2020): 1.1456 - Average: 1.1058 run_config['usd_to_eur'] = (1.0/1.1058) run_config['usd_to_eur'] = 1</pre>	html/eurofxref-graph-

Figure 11: SWIS-100-IE single run jupyter notebook interface

Generic documentation on using the notebook interface is available via the Help menu, and also online²³. In brief, each cell in the notebook contains either a python code fragment or some textual commentary. Code cells can be edited (if desired), and then executed using the Run toolbar button. The typical workflow would be to manually adjust the assignments of one or more run configuration parameters in the run_config data structure, execute the run, and then analyse the results using one or more of the analysis cells provided in the notebook. The available configuration parameters are detailed in Appendix A.3. Results from a run can also be exported to an external spreadsheet file for separate post-processing. This cycle can be repeated as often as desired, to interactively explore different system configurations, within a single notebook session. If desired, additional code or documentation cells can be added. Such modified notebook files may be saved locally, in order to further document (or recreate) specific runs.

2.5.2 Batch run jupyter notebook

The batch run jupyer notebook is called: SWIS-100-single-run.ipynb

Again it will open in a separate browser tab, with a standard jupyter notebook interface as illustrated in Figure 12.

The batch run is driven not by configuration settings specified in the notebook, but by an external spreadsheet file (open document format, extension **.ods**). The SWIS-100-IE distribution includes an example in the file:

batch-run-example/batch_config.ods

This should be copied and edited as appropriate to define the desired set of runs. As with the single run notebook, summary results (for all runs) can be exported to an external spreadsheet file for separate post-processing or analysis.

²³https://jupyter-notebook.readthedocs.io/en/stable/

Jupyter SWIS-100-batch-run Last Checkpoint: 16/02/2021 (autosaved)	ę	Logout
File Edit View Insert Cell Kernel Widgets Help	Trusted	Python 3 O
H K		
SWIS-100 Batch run		
This is an illustrative notebook for running a SWIS-100 "experiment" - a batch of single runs, driven from an array of run configuratio external (hard coded) .ods spreadsheet file. It provides a notebook-based alternative to the command line script version. In particula the <u>mybinder.org</u> cloud service.	ns provided via r, it allows bate	a a single ch runs via
In []: 1 import os 2 import numpy as np 3 import pandas as pd 4 import swisl00 as swis 5		
<pre>In []: 1 batch_configs = pd.read_excel('batch-run-example/batch_config.ods',</pre>		
<pre>In []: 1 batch_configs_dict = batch_configs.to_dict(orient='index') 2 3 display(batch_configs_dict)</pre>		
<pre>In []: 1 batch_dir='batch-run-example'</pre>		



2.5.3 Batch run command line script

Batch runs can also be executed directly from the command line, using the command line script. This is effectively equivalent to simply executing all the code cells in the batch notebook. Accordingly, the required set of configurations must first be set up in an external spreadsheet file, in exactly the same way as already described for the batch notebook. Under the linux command shell, the batch run is then executed by the following command:

./swis100_batch.py <path-to-batch-dir>

where <path-to-batch-dir> denotes the path to a directory (folder) containing the batch configuration file (which must have the name batch_config.ods). The summary results will be stored in the same directory (in a file named batch_stats.ods). Thus, the following command will execute the example batch configuration included in the SWIS-100-IE distribution:

swis100_batch.py batch-run-example

3. Illustrative SWIS-100-IE Runs

This section reviews a series of illustrative runs executed with SWIS-100-IE. These demonstrate the general functionality of the model, and the kinds of output data that can be extracted. Subsections include examples of both single runs and batch runs. These are presented purely as illustrations of the flexible exploration of scenarios for a fully decarbonised (net zero to net negative CO₂ emissions) Irish energy system that is enabled by the tool. They do *not* suggest normative recommendations for any particular policy choices. They do illustrate, in a coarse grained way, that such configurations are *possible in principle*, based on known, existing, technologies; and also serve to give *preliminary* quantitative estimates for the scale of deployment that *might* be required of key technologies, particularly very large scale energy storage and conversion systems that are not required in any substantive way in existing, fossil fuel dominated, energy systems. Much further systematic work is still required to translate these illustrative results into robust findings, and especially to explore *transition* pathways from the current energy system.

3.1 Single run examples

Each illustrative single run uses a common set of parameters as the model complexity allows, building from a the core electricity and energy storage subsystem", onto which Carbon Dioxide Removal (CDR), low temperature heat, surface transport, and air transport are successively added. The key overarching common common parameters for this sequence of single runs are listed in Table 1, while more general technology availabilities are listed in Table 2. Note that nuclear SMR generation was not enabled in any of these single runs and so does not feature in any of the results.

<pre>snapshot_interval (hours)</pre>	12
Nyears	1
assumptions_year	2030
weather_year_start	2010
elec_load_year_start	2014
elec_load_scope	IE
solar_max_p (GW)	3
onshore_wind_max_p (GW)	8.2
offshore_wind_max_p (GW)	inf
<pre>nuclear_SMR_max_p (GW)</pre>	0
IC_max_p (GW)	1.8
IC_max_e (TWh)	0.6048
solar_marginal_cost	0.03
onshore_wind_marginal_cost	0.02
offshore_wind_marginal_cost	0.01
<pre>transport_load_year_start</pre>	2014
heat_year_start	2010
delta_CO2_atm_max (MtCO2)	-5

Table 1: Configuration parameters for illustrative single runs

Nuclear SMR generation	Disabled
Transport technologies	BEV & FCEV
Heating technologies	ASHP & Hydrogen Boiler
Hydrogen Electricity Generation Technology	OCGT & CCGT
Hydrogen Storage Technology	SaltCavern

Table 2: Technology availability for illustrative single runs

3.1.1 Core Electricity and Energy Storage Subsystem

The electricity and energy storage subsystem fully services the electricity end use load (c. 3 GW on average) with no other load connected, with a total system load over the run period of almost 26 TWh. Figure 13 presents sample results of the overall energy balance over the run.



Figure 13: Illustrative single run, core electricity and storage only, overall system energy balance

The primary energy production is fully serviced by wind (8.2 GW onshore and 24 GW offshore) and solar PV (3 GW), with interseasonal storage (hydrogen produced via electrolysis and converted back to electricity via OCGT and CCGT gas turbine generators) filling in the troughs across low sun and wind periods across the year.

Figure 14(a) shows more the detailed energy balance on the electricity bus. Figure 14 (b) focuses in on the electricity bus balance for an example period of high wind availability, while Figure 14 (c)

shows the overall system balance for a period of much weaker wind availability. It is seen that, with high wind availability, interconnector export and hydrogen electrolysis together account for the majority of electricity production which is in excess over immediate concurrent demand at that time. Conversely, in the period of low wind availability, we see that gas turbines (CCGT are OCGT) are dispatched, drawing down stored hydrogen.



Figure 14: Illustrative single run, core electricity and storage only. Detailed energy balances: (a), (b) electricity bus, (c) overall system

All the illustrative single runs have a 12 hour time resolution. At this resolution, battery storage does not feature as a cost-effective storage method, even for diurnal management of solar PV generation, notwithstanding its higher round trip efficiency compared to hydrogen storage. The pattern of energy storage level over the run is shown in Figure 15. The overall capacity factor on the deployed electrolyser infrastructure is less than 17%. The interconnectors and hydrogen storage (almost 3 TWh max) are used in a complementary manner to manage the intermittent periods of primary generation excess or deficit relative to demand across the run. The overall level of dispatch down of available primary generation is <4%.



Figure 15: Illustrative single run, core electricity and storage only, storage utilization over the full run

3.1.2 Addition of Carbon Dioxide Removal (CDR) subsystem

The CDR subsystem is added to the Core Electricity and Energy Storage Subsystem and it imposes a constraint for net removal of CO₂ from the atmosphere and transfer to a secure non-atmospheric store. A negative 5MtCO₂ constraint was added to the model parameters for this single sample run, all other parameters were kept constant.

The overall system balance is shown in Figure 16. This is very similar, as expected because of the same parameters, wind year, technology cost, etc. However direct air capture (DAC) now appears as an additional load to the system; an extra 10.75 TWh, increasing the need for primary energy supply, which is met with deployment of more offshore wind capacity (now 11.37 GW) having already maximised the allowed deployment of onshore wind and solar in meeting conventional electricity demand.



Figure 16: Illustrative single run, core electricity and storage plus 5 Mt CO₂ removal (via DAC), overall system energy balance

Figure 17(a) again shows the more detailed energy balance on the electricity bus. Figure 17(b) focuses in on the electricity bus balance for an example period of high wind availability, while Figure 17(c) shows the overall system balance for a period of much weaker wind availability. It is seen that, with high wind availability, interconnector export and hydrogen electrolysis together account for the majority of electricity production but this is now complemented with significant dispatch of DAC. Conversely, in the period of low wind availability, we see that gas turbines (CCGT are OCGT) are dispatched, drawing down stored hydrogen, and DAC is significantly dispatched down, effectively participating as a demand side management unit (DMU) from the perspective of overall system balance.



Figure 17: Illustrative single run, core electricity and storage plus 5 MtCO₂ removal (via DAC). Detailed energy balances: (a), (b) electricity bus, (c) overall system.

Across the full run duration the DAC performs as expected, with the required 5MtCO₂ moved from the atmosphere and stored permanently as shown in Figure 18, requiring extra primary energy generation of 10.75 TWh, or 2.15 MWh per tCO₂ removed from atmosphere.



Figure 18: Progressive transfer of CO₂ from atmosphere to secure storage via DAC.

3.1.3 Addition of low temperature heat subsystem

The low temperature heat subsystem is added to the Core Electricity and Energy Storage Subsystem and the CDR subsystem; both described previously. With the requirement for more energy supply, from the demand of electricity, seasonal heating and DAC, the system is much larger, at 75.46 TWh, more than double the previous system.

Low temperature heat demand (space and water heating, 38.94 TWh) is characteristically seasonal in Ireland and visible as the large demand across winter and low demand in summer in Figure 19. A more detailed view for an example summer period is shown in Figure 20, and for an example winter period in Figure 21.



Figure 19: Ilustrative single run, core electricity and storage, with CDR and low temperature heating, overall system energy balance



Figure 20: Ilustrative single run, core electricity and storage, with CDR and low temperature heating, overall system energy balance for example summer period.



Figure 21: Ilustrative single run, core electricity and storage, with CDR and low temperature heating, overall system energy balance for example winter period

Figure 22 shows the balance on the (pseudo) low temperature heat bus, showing the breakdown between ASHP and hydrogen boilers. Figure 22(a) shows the full run duration, while Figure 22(b) shows more detail on an example mid-winter peak. It is seen that, for this sample configuration, the deployment of ASHP is the more cost effective option (compared to direct hydrogen combustion) for the majority of space and water heating (38.08 TWh output) due to the substantial energy gain from environmental heat sources. However, to fully cover some short winter peaks coinciding with weak renewable electricity availability, hydrogen boilers are also deployed at a low level (0.86 TWh output).



(b) Winter peak detail

Figure 22: Ilustrative single run, core electricity and storage, with CDR and low temperature heating, heat bus energy balance.

Across the year the DAC performs as required with 5MtCO₂ removed from the atmosphere and stored permanently as shown in Figure 23. However due to the winter bias of heat demand much DAC occurs over summer and into autumn and relatively little in winter periods.



Figure 23: Progressive transfer of CO₂ from atmosphere to secure storage via DAC, interacting with seasonal heat demand.

3.1.4 Addition of surface transport subsystem

The model results present the surface transport subsystem added to the Core Electricity and Energy Storage Subsystem with the CDR subsystem and low temperature heat subsystem, all as described previously. With the requirement for more energy supply, from the demand of electricity, season heating, DAC and transport the system is larger again (88.88 TWh) as shown in Figure 24. A substantial majority is now necessarily derived from offshore wind, with a deployed capacity of 29.7 GW. Surface transport is a very substantial component of overall energy demand in Ireland (13.2 TWh over the run). In this illustrative run, based on the configured underlying technology cost and performance parameters, and the functionally coarse grained options available, battery electric vehicles are generally favoured for deployment over fuel cell electric vehicles for all surface transport. Note that the vehicle fleet is not divided into vehicle duty class, e.g. passenger car or heavy duty vehicle. In practical deployment, the ratio of battery electric vehicle to fuel cell electric vehicle would be significantly affected by this.



Figure 24: Ilustrative single run, core electricity and storage, with CDR, heating, surface transport: overall system energy balance.

3.1.5 Addition of air transport subsystem: full system functionality

As the final single run example, we add the air transport subsystem so that all available components of the SWIS-100-IE model capability are now demonstrated. The system balance, shown in Figure 25, is similar to the previous run, as expected, because of the same parameters, wind year, technology cost, etc., having maximised the allowed deployment of onshore wind and solar.



Figure 25: Ilustrative single run, full SWIS-100-IE functionality: overall system energy balance.

However the total system load is now increased to 96.15 TWh, solar dispatched is 2.78 TWh, onshore wind dispatched is 13.56 TWh and offshore wind makes up the majority of primary energy at 77.62 TWh. Air transport energy demand (for the given example year of 2014) is relatively small compared to heating or surface transport. Nonetheless, because of losses in the Fischer-Tropsch process and additional energy overhead due to DAC (as the source of CO₂), an extra 8 GW of offshore wind capacity was deployed to accommodate the aviation demand.



The impact of air transport on overall hydrogen production and use is shown in Figure 26.

Figure 26: SWIS-100-IE full system, energy balance on the hydrogen bus.

Overall the amount of storage via hydrogen (7.43TWh) and interconnection across the year to accommodate air and surface travel as well as low periods for electricity demand is shown in Figure 27. All the sample model runs have a 12 hour resolution and therefore battery storage does not feature as a cost-effective storage method. Given the cap on storage via interconnection (14 days continuous import/export time at maximum allowed interconnector power capacity) the great majority of storage needs are now satisfied by hydrogen. Overall system dispatch down, even on this substantially expanded system, is still limited to <4%.



Figure 27: SWIS-100-IE full system, energy storage levels across the run.

Figure 28 presents the scale of electricity generation vs demand for the entire system, recognising large peaks of mainly offshore wind producing the large amounts of hydrogen required for storage and the CCGT generators for low periods of renewable availability. Results indicate that for this single run, hydrogen fuelled CCGT was largely deployed in preference to OCGT, the latter being limited to only relatively rare, short, periods of excess of peak demand over supply.



Figure 28: SWIS-100-IE full system, energy balance at the electricity bus.

The DAC infrastructure now integrates both the supply of CO_2 as a feedstock for the Fischer-Tropsch, to produce synthetic aviation fuel, and the (still configured) net transfer of 5MtCO₂/annum from atmosphere to secure storage. The overall CO_2 levels in atmosphere and storage over the run are Figure 29.



Figure 29: SWIS-100-IE full system . Progressive transfer of CO₂ from atmosphere to secure storage via DAC, interacting with seasonal heat demand and synthesis of aviation fuel.

3.2 Batch run examples

3.2.1 Varying time resolution

In this example, we illustrate an investigation of the effect of varying the time resolution in a model configuration. All configuration parameters except for snapshot_interval are given the same values for all runs. The target system is limited to the core Electricity and Energy Storage subsystem (see section 2.2.1CoreSystem]). In summary:

- The run duration is one year.
- Estimated technology parameters refer to a notional "overnight" deployment year of 2030.
- Demand (direct electricity end use) is configured from the historical dataset for 2014, with a scope of Ireland (Republic) only.
- All variable renewable primary energy sources are allowed: solar PV, onshore and offshore wind. The deployable capacities of solar PV and onshore wind are capped. Wind speed and solar insolation data are configured from the historical dataset for 2010. For primary supply dispatch, offshore wind takes priority over onshore wind, which takes priority over solar PV.
- Nuclear electricity generation (SMR) is excluded.
- Deployable interconnector power and remote energy "storage" capacities are both capped. The remote energy storage capacity is set to correspond to a maximum of 14 days continuous running at the maximum deployable power (import or export).
- Both battery and hydrogen energy storage are allowed to be deployed at arbitrary capacities.

The key configuration parameters defining the core system described above are set as shown in Table 3. The batch consists of 5 runs, with the snapshot_interval variable successively set to 1, 3, 6, 12 and 24 hours, i.e. from highest to lowest time resolution. Parameters for the selected historical demand dataset (2014), which do *not* vary with snapshot_interval are shown in Table 4. Conversely, parameters for the historical demand dataset, which *do* vary with snapshot_interval are shown in Table 5. It is noticeable that higher time resolution reveals significantly greater extremes of higher maximum power and lower minimum power.

assumptions_year	2030
Nyears	1
weather_year_start	2010
elec_load_year_start	2014
elec_load_scope	IE
solar_max_p (GW)	3
onshore_wind_max_p (GW)	8.2
offshore_wind_max_p (GW)	inf
<pre>nuclear_SMR_max_p (GW)</pre>	0
IC_max_p (GW)	1.8
IC_max_e (TWh)	0.6048
solar_marginal_cost	0.03
onshore_wind_marginal_cost	0.02
offshore_wind_marginal_cost	0.01

Table 3: Batch run configuration parameters, varying snapshot_interval

local-elec-demand total energy (TWh)	25.771
local-elec-demand mean power (GW)	2.942

	Table 5: Demand	parameters	varving	with sna	pshot	interval
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	01H	03H	06H	12H	24H
local-elec-demand max power (GW)	4.573	4.301	4.083	3.985	3.530
local-elec-demand min power (GW)	1.684	1.723	1.797	2.084	2.315

Following execution of the batch runs, the summary output data is available in a spreadsheet file (named batch_stats.ods by default). The deployed VRE generation power capacities are shown in Table 6. It is found that the power capacities of Solar PV, onshore Wind, and interconnector all reach their maximum allowed values, per the input configuration constraints, for all snapshot_interval values. The only one which varies is offshore wind, and even then the variation is relatively small. The power capacities of the firm (dispatchable) generation components (from all forms of storage, including interconnection) are shown in Table 7. It is seen that battery generation is deployed only when the system is solved with a snapshot_interval of 01H or 03H, showing that (on the basis of the configured notional cost assumptions) battery storage is only cost effective for energy time arbitrage, relative to the hydrogen-based alternatives, for small storage times. It is also notable that, at high time resolution, even with the deployment of significant

battery capacity, the other firm generation capacities are also increased (hydrogen OCGT and CCGT), so that total firm capacity is significantly higher. Comparing with the maximum demand data in Table 5 it is evident that the greater peak power demand revealed at high time resolution is primarily satisfied by deploying this combination of greater firm power capacities (mediated by storage) as opposed to any significantly greater primary VRE capacity deployment.

	01H	03H	06H	12H	24H
solar capacity nom (GW)	3.000	3.000	3.000	3.000	3.000
onshore wind capacity nom (GW)	8.200	8.200	8.200	8.200	8.200
offshore wind capacity nom (GW)	5.406	5.406	5.378	5.245	5.003
Total VRE capacity (GW)	16.606	16.606	16.578	16.445	16.203

Table 6: Deployed power capacities of variable renewable electricity generation

Table 7: Deployed power capacities of firm electricity generation

	01H	03H	06H	12H	24H
IC power (GW)	1.800	1.800	1.800	1.800	1.800
H2 OCGT o/p capacity (GW)	0.991	0.997	0.716	0.748	0.342
H2 CCGT o/p capacity (GW)	1.125	1.151	1.163	1.013	0.729
Battery power capacity (GW)	0.452	0.132	0.000	0.000	0.000
Total Firm capacity (GW)	4.368	4.080	3.679	3.561	2.870

Table 8 shows the deployed *energy storage* capacities. The modelled storage associated with the remote grid interconnection was constrained to a maximum cumulative imbalance of 14 days at full power import or export, and this is fully deployed in all cases. Note that the battery energy capacity is shown in units of GWh, whereas the hydrogen store and the storage represented by the interconnection are expressed in units of TWh. This emphasises that while some significant battery storage is deployed when the system is solved at high time resolution (01H or 03H), and the power capacity is very important to meet peak power demands at this time resolution, it is only found (notionally) cost-effective for such relatively short duration running. Far the most dominant demand on storage is for longer time periods, and is already evident even when the system is solved with relatively low time resolution of 12H or even 24H. The *total* deployed energy storage capacity, and varies only to a relatively small extent with varying time resolution. Finally it may be noted that the even the maximum battery deployment (at 01H time resolution) is broadly comparable to the pumped hydro storage (in both power and energy) already physically deployed in the Irish electricity system²⁴, but not explicitly modelled in SWIS-100-IE.

²⁴https://esbarchives.ie/portfolio/turlough-hill/

	01H	03H	06H	12H	24H
Battery store (GWh)	1.130	0.440	0.000	0.000	0.000
H2 store (TWh)	2.272	2.274	2.254	2.254	2.310
Remote grid 'store' (TWh)	0.605	0.605	0.605	0.605	0.605
Total storage (TWh)	2.878	2.879	2.859	2.859	2.915

Table 8: Deployed energy storage capacities

3.2.2 Varying weather year

In this example, we illustrate an investigation of the effect of varying the choice of weather year (determining the specific historical variability in VRE generation capacity factor) in a model configuration. All configuration parameters except for weather_year_start are given the same values for all runs. The snapshot_interval is set to 06H and the target system is otherwise configured in the same way as the previous batch run example (see section 3.2.1), as shown in Table 9.

assumptions_year	2030
Nyears	1
<pre>snapshot_interval</pre>	6
elec_load_year_start	2014
elec_load_scope	IE
solar_max_p (GW)	3
onshore_wind_max_p (GW)	8.2
offshore_wind_max_p (GW)	inf
<pre>nuclear_SMR_max_p (GW)</pre>	0
IC_max_p (GW)	1.8
IC_max_e (TWh)	0.6048
solar_marginal_cost	0.03
onshore_wind_marginal_cost	0.02
offshore wind marginal cost	0.01

Table 9: Batch run configuration parameters, varying weather year

The batch consists of 5 runs, with the weather_year_start parameter successively set to 2010, 2011, 2012, 2013 and 2014. Each run represents a duration of one year, so there is no time overlap between the runs. It is important to reiterate that these runs apply *myopic* optimisation: the system is constrained in such a way that all the final energy in a given run must be derived from primary energy generated within that run: there is no net change in any energy store (including no net interconnector import or export) over the run, and thus no net time arbitrage of energy on any time scale longer than the run. Thus, the outputs represent a notional "steady state" optimisation that is implicitly premised on exactly the same load and weather pattern repeating indefinitely. Practical system configuration would, of course, have to take a prudential view that would have sufficient overcapacity coupled with year on year energy arbitrage to deal with the large scale variability in VRE supply, rather than simply optimising for one particular weather year.

All runs in this batch use the same historical demand dataset (2014). Key overall demand parameters are shown in Table 10, evaluated for the given snapshot_interval (06H) where relevant.

local-elec-demand total energy (TWh)	25.771
local-elec-demand mean power (GW)	2.942
local-elec-demand maximum power (GW)	4.083
local-elec-demand minimum (GW)	1.797

Table 10: Batch run demand parameters, varying weather year

Table 11: Nominal VRE capacity factors, varying weather year

Nominal (max) capacity factors (%)	Weather-2010	Weather-2011	Weather-2012	Weather-2013	Weather-2014
solar PV	10.9	10.1	9.7	10.1	10.5
onshore wind	22.4	30.7	27.4	29.4	27.7
offshore wind	23.7	31.9	29.7	30.4	29.5

Table 12: Achieved VRE capacity factors, varying weather year

Achieved capacity factors (%)	Weather-2010	Weather-2011	Weather-2012	Weather-2013	Weather-2014
solar PV	10.5	9.5	9.1	9.4	10.1
onshore wind	20.7	29.6	26.1	28.3	26.4
offshore wind	23.7	31.9	29.7	30.4	29.5

The key variation in this batch is in the underlying availability of VRE primary energy (for any given capacity deployment). This is manifested through the high time resolution datasets for nominal capacity factor (in the absence of dispatch down). The nominal capacity factors for the distinct VRE technologies, averaged over each run, are shown in Table 11. It is seen that, over this particular sample of five years, there is relatively little variation in solar energy nominal capacity factor (averaged over each full year), but very significant variation in wind energy nominal capacity factor, both onshore and offshore; 2010 was evidently an especially poor wind year, both onshore and offshore and offshore in this batch run.

The actually achieved average capacity factors for each run (now inclusive of dispatch down, under notional cost optimisation) are shown in Table 12. Because of the chosen dispatch priority (first offshore wind, then onshore wind, then solar), offshore wind achieves its full nominal capacity factor (essentially zero dispatch down); whereas there is some modest dispatch down of both onshore wind and solar PV, with corresponding reductions in achieved capacity factors. However, the effect is very modest, and the overall situation is still essentially reflective of the especially poor wind conditions in 2010 relative to the other four years.

The deployed power generation capacities of the primary VRE sources are shown in Table 13; and the capacities of firm (dispatchable) generation components (from all forms of storage, including interconnection) are shown in Table 14. Note that no battery generation is shown as, at the chosen time resolution (06H) there is no cost-effective deployment of battery storage.

	Weather-2010	Weather-2011	Weather-2012	Weather-2013	Weather-2014
solar PV capacity nom					
(GW)	3.000	3.000	3.000	3.000	3.000
onshore wind capacity					
nom (GW)	8.200	8.200	8.200	8.200	8.200
offshore wind capacity					
nom (GW)	5.378	1.958	2.663	2.170	2.906
Total (GW)	16.578	13.158	13.863	13.370	14.106

Table 13: Deployed VRE power capacities, varying weather year

Table 14: Deployed firm power capacities, varying weather year

	Weather-2010	Weather-2011	Weather-2012	Weather-2013	Weather-2014
IC power (GW)	1.800	1.800	1.800	1.800	1.800
H2 OCGT o/p					
capacity nom (GW)	0.716	0.753	0.713	0.991	0.976
H2 CCGT o/p					
capacity nom (GW)	1.163	1.204	1.134	1.033	1.057
Total (GW)	3.679	3.757	3.647	3.824	3.832

Table 15: Deployed energy storage capacities, varying weather year

	Weather-2010	Weather-2011	Weather-2012	Weather-2013	Weather-2014
Remote grid 'store' (TWh)	0.605	0.605	0.605	0.605	0.605
H2 store (TWh)	2.254	2.613	1.184	1.865	2.893
Total (GW)	2.859	3.218	1.789	2.469	3.498

It is seen that, based on the demand profile (common for all runs), the relatively lower cost solar PV and onshore wind primary VRE sources are deployed at the maximum allowed capacities in all cases, and only offshore wind capacity varies. However, this variation is very significant, ranging from a minimum of 1.96GW in the "best" wind year (2011) to a maximum of 5.38GW in the "worst" year (2010); a ratio of over 2.7:1. But although 2010 was clearly exceptional, even across the other four years, the ratio from maximum to minimum is still almost 1.5:1. It is evident that, for a system dominated by VRE primary energy sources, prudential capacity planning may require significant over-provisioning relative to "average" annual yield; although this may be substantially moderated if there is well functioning, large scale, international trade in zero-emissions energy carriers over sufficiently large temporal and geographical ranges (to overcome regional correlations in VRE yields). This is at least suggestive of the potential strategic importance of both "green" hydrogen and "green" ammonia (derived from green hydrogen), to facilitate such trade, including both transport and storage at very large scales.

Finally, Table 15 shows the deployed *energy storage* capacities. As already noted, with 06H time resolution, there is no role for battery storage, and it is omitted. Similarly to the previous batch run example (section 3.2.1), the modelled storage associated with the remote grid interconnection was constrained to a maximum cumulative imbalance of 14 days at full power import or export, and this is fully deployed in all cases. Accordingly the only variation in storage capacity is in relation to the

hydrogen store. It is notable that this (myopically optimised) hydrogen storage capacity also shows very significant variation according to the varying weather profile: from a minimum of 1.18TWh (in 2012) to a maximum of 2.89TWh (in 2014); a ratio from maximum to minimum of more than 2.5:1. It also evident that, unlike the case of raw VRE power generation capacity, there is no simple correlation here between storage deployment and *average* weather (especially wind) conditions. Notionally optimal storage deployment is evidently (and understandably) more sensitive to the higher resolution temporal structure of the weather conditions over the year, rather than the year long average.

4. Future Work

The previous report sections have documented the motivation, architecture, and use of the initial release of the SWIS-100-IE model. In summary, it is already fully usable for the quantitative exploration of scenarios for the future configuration of the Irish energy system, premised on primary reliance on *unequivocally* zero emissions energy sources (excluding embodied emissions in infrastructure). Nonetheless, there are also significant omissions and limitations in the current functionality. This section outlines some specific planned directions for future development and application of the tool.

The most immediate limitation of SWIS-100-IE is that it is not suitable to explore *intermediary* configurations *between* the current (fossil fuel dominated) energy system and potential future, fully decarbonised system configurations. Within the coarse grained framework of the tool, this can be addressed by adding a small number of additional components:

- Fossil fuelled electricity generation. Given the imminent retirement of most fossil fuel electricity generation in Ireland other than using fossil ("natural") gas, it is likely sufficient to add support for fossil gas fired generation, coupled appropriately with the existing SWIS-100-IE CO₂ tracking functionality. At most four variations are likely appropriate: OCGT or CCGT, each with or without CCS: that is, four additional, aggregated, generator components, each with configuration options for minimum and maximum deployed capacity. It will also be necessary to add assumptions on fossil gas fuel cost.
- Combustion engine (ICE) surface transport. This can be added as an additional link component, representing a notional ICE fleet, in parallel with the existing BEV and FCEV links. This is essentially analogous to the existing Aircraft link, including the emission of CO₂ to the atmospheric store. It would have configuration options for minimum and maximum deployed capacity. In addition to the existing zero-carbon liquid hydrocarbon *synthesis* pathway, a direct "generator" of (fossil) liquid hydrocarbon is also required, with associated assumptions on costs of such fuel. Both surface and air transport would thus have access to a fossil fuel pathway as well as synthetic fuel pathway. There is also an argument for splitting surface transport demand between heavy and light duty vehicles, given the significant different technology parameters (especially FCEV vs BEV) that would be properly applicable in each case.
- Fossil fuel supply of low-temperature heat. Additional links, representing notional (aggregate) fossil gas and fossil liquid fuelled boilers, can be added in parallel with the existing ASHP and H₂ boiler links. As with the addition of ICE transport, these would include emission CO₂ to the atmospheric store, and would each have configuration options for minimum and maximum deployed capacity.
- While the hydroelectricity resource (including pumped hydro storage) in Ireland is relatively limited, nonetheless it has the significant advantage of offering some firm electricity generation capacity with zero CO₂ emissions and at comparatively low (largely already sunk) cost. Thus, it would be useful to add this, still in a suitably coarse grained, nationally aggregated, manner.

With these additional components in place, and in the absence of any constraint on CO₂ increase in the atmospheric store, the notional cost optimisation of deployed capacities will yield a fossil-fuel dominated configuration. With appropriate constraints on specific components, this can be calibrated to (coarsely) match the current system configuration. Intermediate configurations toward decarbonisation can then be investigated by progressively imposing a constraint on net increase in

CO₂ to the atmospheric store. In the way, outline *decarbonisation pathways* may be constructed, based on a prescribed reduction pathway for CO₂ emissions rate at each intermediate step. Such an investigation would be methodologically similar to that previously undertaken by (Connolly and Mathiesen 2014); but with the significant advantages of supporting notional cost optimisation of deployed capacities at each intermediary configuration. It would also offer additional major options (including nuclear energy supply, synthetic liquid fuel supply for aviation and capability for net-negative CO₂ emissions), be focussed on transition to *unequivocally* zero emissions energy sources and be implemented on a fully open source code platform, using open datasets of demand, weather, and technology parameters.

A final (more demanding) development would be to provide integration of such discrete step pathways, with a *cumulative* emissions framework, to satisfy a specific "national cumulative-GHG quota" (NCQ) (McMullin et al. 2019). This is a central requirement to show explicit and transparent alignment of any proposed national decarbonisation pathway with a "fair share contribution" to meeting the temperature goals of the Paris Agreement (UNFCCC 2015) (Rogelj et al. 2021).

5. Conclusion: Innovation/Novelty – Beyond State-ofthe-Art

A new modelling tool, denoted SWIS-100-IE, has been developed to support to exploration of prospective future configurations of the Irish Energy system, based on the use of *unequivocally* zero-CO₂ energy sources (wind, solar and nuclear), with the additional option of requiring removal of CO₂ from atmosphere to secure, long term, storage (CDR). While acknowledging that deployment of nuclear energy is currently prohibited by statute in Ireland, this is subject to ongoing societal debate. Both the inclusion of nuclear on the basis of projected availability of small modular reactors, and the provision for technological CDR, are considered as novel and represent advances on the prior state of the art.

SWIS-100-IE is characterised as functionally coarse grained but temporally fine grained. That is, the framework is deliberately designed to offer only a simplified, schematic, set of system configuration options. All major elements are aggregated at a national level (demand sectors, energy sources, storage and conversion systems). This facilitates tractable (even interactive) exploration of the large scale space of strategic approaches to Ireland's future energy system, including the ability to investigate the general structure of interactions between the major functional choices. However: it is temporally fine grained (potentially down to one-hour time resolution, over periods of up to c. five years). This is essential to meaningfully represent the interactions in time between varying energy sources, energy demands and energy storage. This combination of functional coarse graining with temporal fine graining in a model tailored to Irish energy system resources and demand is novel, and an advance on the prior state of the art.

SWIS-100-IE integrates a suite of historical demand datasets, covering conventional electricity use, low temperature (space and water) heating and transport (surface and air). It also incorporates historical datasets for key weather related variables: wind speed, solar insolation, air temperature. The incorporation of (externally developed) synthetic, high time resolution, timeseries for low temperature heat demand, and with estimates of real-time heat pump co-efficient of performance (when2heat) is believed to be novel and unique in current Irish energy system modelling.

SWIS-100-IE incorporates support for decarbonisation of aviation via the production of synthetic aviation fuel (chemically conventional liquid hydrocarbon jetfuel) from feedstocks consisting of (green) hydrogen and CO₂ directly removed from air. This ensures complete closure of the carbon flow (within the duration of the run), hence zero net emission of CO₂ to atmosphere, without reliance on currently speculative new aircraft propulsion technologies, or biofuels (with highly contested emissions impacts), or conventional "offsets" (largely discredited in the forms deployed to date). In itself, this still does not address the non-CO₂ climate forcing arising from aviation, which is comparatively more uncertain than the direct CO₂ forcing. However, such effects can be separately compensated within SWIS-100-IE by deployment of a corresponding (exogenously determined) amount of additional CDR. Such physically monitored and verified material compensation of climate forcing is not subject to the defects of conventional "offsetting". Taken together, these model approaches to full decarbonisation of aviation energy (delivered to aircraft refuelled in Ireland) are also believed to be novel and unique in Irish energy system modelling.

SWIS-100-IE is a so-called "capacity expansion" model: it attempts to automatically identify the "notionally optimal" sizes of all major infrastructural elements in order to meet the specified sectoral demand profiles over the full period of any given run. This is contingent on an included database of notional capital cost estimates (and other relevant technical parameters) for each supported

technology. While optimal capacity expansion is not unique to this model, its application in the context of high time resolution demand and weather data, with exclusively zero-CO₂ energy sources is considered to be novel, and distinct from the prior state of the art.

In keeping with the overarching commitment to open development underpinning the OESM-IE project, SWIS-100-IE has been developed using only tools and datasets that, as far as possible, are available under permissive open licencing. SWIS-100-IE itself is released under the GNU General Public License Version 3²⁵. SWIS-100-IE is developed to be platform-neutral as far as possible. That is, it will be possible to install and execute experiments on conventional local computing platforms, (open or proprietary: linux, Microsoft Windows, macOS). In addition, SWIS-100-IE is configured to support deployment on the mybinder open, cloud-based, platform. This facility for cloud based execution of an open energy system model is believed to be novel in the Irish context, and certainly reflects the most advanced state of the art for such work.

²⁵https://www.gnu.org/licenses/gpl-3.0.en.html

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Appendices

A.1 Project RDD246: Original WP3 Summary

WP No. & Title	WP3: Develop negative-CO2 energ	y system scenarios		
Start Month No.	6	Finish Month No.	11	
WP Lead:	DCU			
WP Contributors	N/A			
Objective(s)	WP3-O1: Develop and characterise system configurations.	e a range of negative-CO	2 scenarios and energy	
Description (max 200 words)	Based on the baseline OESM-IE from WP2, this WP will go on to design and implement at least one potential future negative-CO ₂ configuration for the Irish energy system. This will be used to specifically investigate the interacting roles of: demand constraint (via efficiency measures or otherwise), degree of electrification (of heating and transport), VRE, bioenergy, energy storage, bio- and synthetic fuel and CO ₂ cycle pathways including geological CO ₂ storage (role of CCS). It will investigate and characterise the role of heterogenous energy storage, in particular the interactions between overall system electrification, VRE penetration, and use of bio- and synthetic-fuels (gaseous and liquid) both as energy stores and as direct fossil fuel substitutes in the most difficult to electrify transport and heating applications (respectively, aviation and shipping, and high temperature process heating).			
Milestones	WP3-M1: Demonstration and characterisation of a range of negative-CO ₂ configurations in OESM-IE.			
Deliverables	 WP3-D1: Negative-CO₂ OESM-IE configuration with full datasets. WP3-D2: Technical report documenting negative-CO₂ OESM-IE configuration and characterising roles of heterogenous energy storage and electrification. WP3-D3: Submission of associated paper for peer-reviewed journal publication. 			

A.2 Software and datasets: Open Release

The SWIS-100-IE modelling platform, and the associated technology database, has been released via the github open source development service. It may be accessed at the following URL:

https://github.com/bmcmullin/SWIS-100-IE/tree/master

More detailed instructions on downloading, installing and executing the model, and all required external datasets, are provided in sections 2.4 and 2.5 of the main body of the report.

A.3 SWIS-100-IE configuration parameters

The following table briefly describes all the configuration parameters available with the initial release of SWIS-100-IE.

ASHP_max_p (GW)	Air source heat pump (aggregate component): maximum deployable input power capacity.
ASHP_min_p (GW)	Air source heat pump (aggregate component): minimum deployable input power capacity.
BEV_max_p (GW)	Battery electric surface vehicle fleet (aggregate component): maximum deployable input power capacity.
BEV_min_p (GW)	Battery electric surface vehicle fleet (aggregate component): minimum deployable input power capacity.
Battery_max_e (MWh)	Grid battery storage system: maximum deployable energy capacity.
Battery_max_p (MW)	Grid battery storage system: maximum deployable power (input and output) capacity.
delta_CO2_atm_max (MtCO2)	Maximum allowed change (delta) in the level of atmospheric CO_2 over the run (relative to baseline zero prior to run start); equivalent to net cumulative CO_2 emissions from all sources over the run. Set <i>negative</i> to force net CO_2 removal from atmosphere (CDR) over the run.
FCEV_max_p (GW)	Hydrogen fuel cell electric surface vehicle fleet (aggregate component): maximum deployable input power capacity.
FCEV_min_p (GW)	Hydrogen fuel cell electric surface vehicle fleet (aggregate component): minimum deployable input power capacity.
H2_CCGT_max_p (GW)	Hydrogen-fuelled combined cycle gas turbine electricity generator fleet (aggregate component): maximum deployable input (hydrogen) power capacity. Note carefully that the consequent limit on <i>output</i> power (as electricity) will be this value derated by the nominal CCGT conversion efficiency specified in the technology database.
H2_OCGT_max_p (GW)	Hydrogen-fuelled open cycle gas turbine electricity generator fleet (aggregate component): maximum deployable input (hydrogen) power capacity. Note carefully that the consequent limit on <i>output</i> power (as electricity) will be this value derated by the nominal OCGT conversion efficiency specified in the technology database.

H2_boiler_max_p (GW)	Direct combustion hydrogen boiler fleet (aggregate component) for production of low-temperature heat: maximum deployable input (hydrogen) power capacity.
H2_boiler_min_p (GW)	Direct combustion hydrogen boiler fleet (aggregate component) for production of low-temperature heat: minimum deployable input (hydrogen) power capacity.
H2_electrolysis_max_p (GW)	Hydrogen electrolyser fleet (aggregate component) for production of hydrogen from electricity: maximum deployable input (electricity) power capacity.
H2_electrolysis_tech	Hydrogen electrolyser fleet technology. See the technology database for technology options and corresponding parameters.
H2_storage_tech	Hydrogen storage technology. See the technology database for technology options and corresponding parameters.
H2_store_max_e (TWh)	Hydrogen energy storage system: maximum deployable <i>energy</i> capacity.
IC_max_e (TWh)	Interconnection is crudely modelled as a form of temporary energy "storage" on the remote side. This parameter sets the maximum deployable remote energy storage capacity. Note that total import and export over the full run is separately required to balance. This means that the final level of notionally stored energy (on the remote side of the interconnector) must be the same as the initial value: but the specific initial level is optimised relative to the deployed storage capacity.
IC_max_p (GW)	Interconnector (aggregate component): maximum deployable power capacity – limits import and export, as measured on the local grid side.
IC_min_p (GW)	Interconnector (aggregate component): minimum deployable power capacity – limits import and export, as measured on the local grid side.
Nyears	Number of years for the model run. Integer (runs must span an integer number of years). Solving time will go up non-linearly with the number of years and the time resolution (see configuration parameter snapshot_interval). It is generally recommended not to set this to more than 5.
assumptions_year	Calendar reference year for setting technology parameters, including notional costs. Must be 2020, 2030 or 2050.

constant_air_transport_load (GW)	If the configuration variable constant_air_transport_load_flag is True then the final (mechanical energy) air transport load power for the run will be constant, at this level. The level may be set to zero to effectively omit all air transport load.
constant_air_transport_load_flag	Boolean flag. If True then the final (mechanical energy) air transport load power for the run will be constant, at the level determined by the configuration parameter constant_air_transport_load (GW). If False, the final air transport load power for the run will match an historical dataset beginning at the start of the year determined by the configuration parameter transport_load_year_start.
constant_elec_load (GW)	If the configuration parameter constant_elec_load_flag is True then the direct electricity load power for the run will be constant, at this level. The level may be set to zero to effectively omit all direct electricity load.
constant_elec_load_flag	Boolean flag. If True then the direct electricity load power for the run will be constant, at the level determined by the configuration parameter constant_elec_load (GW). If False, the direct electricity load power for the run will match an historical dataset beginning at the start of the year determined by the configuration parameter elec_load_year_start.
<pre>constant_lo_temp_heat_load (GW)</pre>	If the configuration parameter constant_lo_temp_heat_load_flag is True then the final low temperature heat load power for the run will be constant, at this level. The level may be set to zero to effectively omit all low temperature heat load.
constant_lo_temp_heat_load_flag	Boolean flag. If True then the final low temperature heat load power for the run will be constant, at the level determined by the configuration parameter constant_lo_temp_heat_load (GW). If False, the final low temperature heat load power for the run will match a synthetic historical dataset beginning at the start of the year determined by the configuration parameter heat_year_start.
constant_surface_transport_load (GW)	If the configuration parameter constant_surface_transport_load_flag is True then the final (mechanical energy) air transport load power for the run will be constant, at this level. The level may be set to zero to effectively omit all surface transport load.

constant_surface_transport_load_f lag	Boolean flag. If True then the final (mechanical energy) surface transport load power for the run will be constant, at the level determined by the configuration parameter constant_surface_transport_load (GW). If False, the final surface transport load power for the run will match an historical dataset beginning at the start of the year determined by the configuration parameter transport_load_year_start.
elec_load_scope	Geographical scope of historical dataset for direct electricity load. Applicable only if the configuration parameter constant_elec_load_flag is False. Allowed values are as follows: IE selects Republic of Ireland only, NI selects Northern Ireland only, IE+NI selects all island (Republic of Ireland plus Northern Ireland).
elec_load_year_start	Start year of historical dataset for direct electricity load. Applicable only If the configuration parameter constant_elec_load_flag is False. The end year will be elec_load_year_start + (Nyears - 1). Datasets are available for each year in the range 2014-2019 inclusive: both start and end years must fall within this range. The geographical scope of the dataset is set by the configuration parameter elec_load_scope.
heat_year_start	Start year of synthetic historical dataset for both the synthetic historical low temperature heat load and the (time varying) synthetic historical COP values for the ASHP (air source heat pump) Link component. Applicable only if the configuration parameter constant_lo_temp_heat_load_flag is False.The end year will be heat_year_start + (Nyears - 1). Datasets are available for each year in the range 2008-2013 inclusive: both start and end years must fall within this range. See (Ruhnau et al. 2019) for methodological details of the derivation of the source datasets.
nuclear_SMR_max_p (GW)	Small nuclear reactor (SMR) electricity generator fleet (aggregate component): maximum deployable output (electricity) power capacity.
nuclear_SMR_min_p (GW)	Small nuclear reactor (SMR) electricity generator fleet (aggregate component): minimum deployable output (electricity) power capacity.

offshore_wind_marginal_cost	Notional marginal cost of each unit (€/MWh) of electricity output from the aggregate offshore wind generator fleet. The only function of this is to indicate dispatch priority relative to other VRE electricity generators (onshore wind and solar PV). Normally configured with a nominal value (less than €0.05). See also: onshore_wind_marginal_cost and solar_marginal_cost.
offshore_wind_max_p (GW)	Offshore wind electricity generator fleet (aggregate component): maximum deployable output (electricity) power capacity.
offshore_wind_min_p (GW)	Offshore wind electricity generator fleet (aggregate component): minimum deployable output (electricity) power capacity.
onshore_wind_marginal_cost	Notional marginal cost of each unit (€/MWh) of electricity output from the aggregate onshore wind generator fleet. The only function of this is to indicate dispatch priority relative to other VRE electricity generators (offshore wind and solar PV). Normally configured with a nominal value (less than €0.05). See also: offshore_wind_marginal_cost and solar_marginal_cost.
onshore_wind_max_p (GW)	Onshore wind electricity generator fleet (aggregate component): maximum deployable output (electricity) power capacity.
onshore_wind_min_p (GW)	Onshore wind electricity generator fleet (aggregate component): minimum deployable output (electricity) power capacity.
snapshot_interval	Size of each time step for run, in hours. Integer. Should be some integral divisor of 24 hours: 1, 2, 3, 4, 6, 12, 24. Solving time will go up non-linearly with the time resolution (smaller snapshot_interval) and with the number of years (see configuration parameter Nyears).
solar_marginal_cost	Notional marginal cost of each unit (€/MWh) of electricity output from the aggregate solar PV generator fleet. The only function of this is to indicate dispatch priority relative to other VRE electricity generators (onshore and offshore). Normally configured with a nominal value (less than €0.05). See also: onshore_wind_marginal_cost and offshore_wind_marginal_cost.
solar_max_p (GW)	Solar PV generator fleet (aggregate component): maximum deployable output (electricity) power capacity.

solar_min_p (GW)	Solar PV generator fleet (aggregate component): minimum deployable output (electricity) power capacity.
solver_name	Name of preferred external LP solver. Normally either cbc or glpk.
transport_load_year_start	Start year of historical dataset for the surface and/or air transport loads. Applicable only if the respective "constant load" configuration parameter (constant_surface_transport_load_flag or constant_air_transport_load_flag) is False.The end year will be transport_load_year_start + (Nyears - 1). Transport load datasets are available for each year in the range 1991-2017 inclusive: both start and end years must fall within this range.
usd_to_eur	Certain costs in the supplied technology parameter database are expressed in US dollars (USD). These are converted to Euro (EUR) values by multiplying by this conversion factor.
weather_year_start	Start year of historical dataset for onshore and offshore wind and solar PV capacity factors. Datasets are normalised to a maximum of 1.0 and incorporated as time varying per unit capacity factors (PyPsa parameter p_max_pu) in the corresponding generator components. Datasets represent averaged values over the relevant geographical areas (Irish onshore or offshore territory). The end year will be weather_year_start + (Nyears - 1). Weather datasets are available for each year in the range 1985-2015 inclusive: both start and end years must fall within this range. See (Staffell and Pfenninger 2016) and (Pfenninger and Staffell 2016) for methodological details of the derivation of the source datasets.