Energy Technology Systems Analysis Programme

ETSAP Project Report

Improving the modelling of Energy Storage Technologies in TIMES via collaboration with TCP Energy Storage Annex 32

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1. INTRODUCTION

In 2020, IEA Energy Storage (ES TCP) started a new project to develop an open-source modelling platform for energy storage under Task 32, managed by Prof. Dr-Ing. Christian Doetsch from the Fraunhofer UMSICHT institute in Germany. Given the strong emergence of storage technologies in deep decarbonisation scenarios in TIMES, it was considered that a collaborating with ES TCP Task 32 and ETSAP, including exchanging knowledge on methodologies and data, would be of mutual interest.

1.1 ES TCP Task 32: Objectives and structure

Task 32 aimed to create open-source models and data sets for energy storage. It created mathematical descriptions of storage technologies on two levels of detail. The first level, called L1, is based on linear constraints, while the second level, called L2, introduces non-linear effects in storage operations. Also, Task 32 provided test cases of the developed models. TIMES was part of the L1 suite of models of Task 32.

Task 32 was divided into three subtasks: Subtask 1 (ST-1), Subtask 2 (ST-2), and Subtask 3 (ST-3); see Figure 1. ST-1 dealt with input data collection for the energy storage models. ST-2 focused on the development of models for electrical and thermal energy storage. ST-3 provided test cases of the models developed in ST-2.

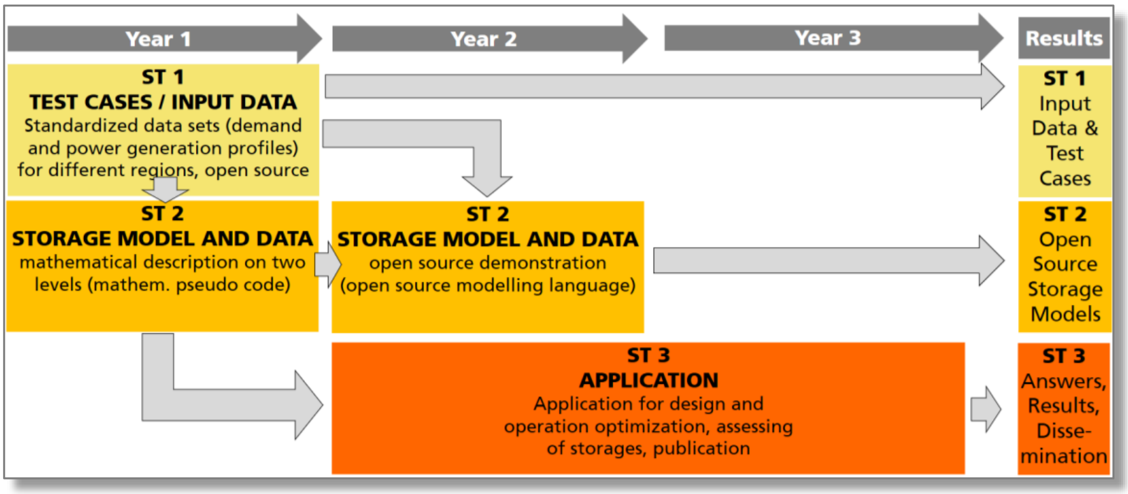

Figure 1: Organisational structure of Task 32 and its time plan (Doetsch et al., 2024)

Each subtask had a leader who organised meetings and coordinated with other subtask leaders. Regular meetings were held to discuss progress, address challenges, and exchange ideas. Yvonne Scholz from DLR (Germany) coordinated ST-1, Claudio Brivio from CSEM (Switzerland) was the head of the electricity energy storage models in ST-2, and Ian Beausoleil Morrison from Carleton University (Canada) led the thermal storage models in ST-2. The applications of the ST-2 models in ST-3 were coordinated by Qianpu Wang (for large-scale applications) and Natesa MacRae (small-scale applications), both from NRC (Canada) with assistance from Alireza Afshari from Aalborg University (Denmark).

1.2 Aims of the collaboration between ETSAP and ES TCP Task 32

The collaboration aimed to explore potential synergies between the two TCPs, which is at the heart of the TCP activity of IEA. ETSAP aimed to benefit from the storage technology expertise in Task 32 to improve the mathematical description of storage technologies in TIMES and, potentially, to enhance the ETechDS database platform with the data collected within ES TCP Task 32.

ES TCP Task 32 sought to learn more about the energy storage modelling in TIMES, and have TIMES models as a platform for using the data collected in Task 32. At the same time, Task 32 aimed to gain more insights into the role of storage in low-carbon energy systems worldwide through the very rich set of energy systems decarbonisation studies performed with TIMES models worldwide.

Hence, the collaboration between ETSAP and ES TCP Task 32 focused mainly on ST-2 (modelling of storage) and ST-3 (case studies and dissemination) activities.

1.3 Summary of the main outcomes from ETSAP and Task 32 collaboration

Below is a summary of the outcomes of Task 32 that are of relevance to the ETSAP community:

- Exchanges on the methodology and data in storage modelling between ETSAP and ES TCP ES Task 32. This was done through a joint workshop to improve the awareness among the two TCPs. In addition, TIMES presentations on storage modelling and applications were presented in meetings with ES TCP Task 32.
- Open-source datasets related to modelling energy storage technology, including GIS-based renewable energy potentials, timeseries of renewable energy, electricity load and heat loads, electricity prices, etc. for several world regions. In addition, real-case storage operation data were collected. These datasets were complemented by the latest storage technology costs and performance estimates.
- Open-source models for the operation of energy storage technologies that capture also non-linear effects, such as battery degradation. These models operate at very high spatial resolution (e.g. individual storage technologies or buildings and districts) and a very high temporal resolution (e.g., from seconds

to hours). Therefore, they need to be carefully considered before assessing the possibility of integrating some of their features in TIMES since TIMES models have linear formulations of the storage technical constraints and operate at much coarser spatial and temporal resolutions.

In addition, this activity triggered the development of a SubRES template for modelling different storage technologies in TIMES models. This is also attached to the current report.

2. Relevance of ETSAP-TIMES to ES TCP Task 32

2.1 Introducing TIMES and its applications to the ES TCP Task 32

This first collaborative activity included two presentations of TIMES to ES TCP Task 32.

The first presentation (jointly delivered by P. Seljom and E. Panos on 03.12.2020) gave insights into the role of energy storage in future energy systems based on analyses with TIMES models worldwide. The presentation is attached to this report in the file: **ETSAP_TIMES_ST3_20201203.pdf** (Panos et al., 2020)).

Seven case studies with TIMES were highlighted in this presentation and provided by several ETSAP teams. The presentation highlighted the richness of the insights gained with the TIMES framework regarding the future role of storage technologies. At the same time, it demonstrated the challenges in representing storage within energy systems models.

For example, the role of storage technology in the future energy system was highlighted in the following cases:

- In decarbonisation scenarios for **Canada** (Vaillancourt & et. al, 2016)
- In decarbonising the **European** power sector (Golombek et al., 2022)
- In the power sector of **Portugal** (https://clim2power.com)
- In the **Swiss** energy system (Panos et al., 2019)

At the same time, advanced modelling methodologies to better capture the role of energy storage in large-scale energy systems models were discussed, including:

- Role of **asymmetric timeslices** in energy storage investments (Hamasaki & Kanudia, 2019); see also Figure 3
- Role of **stochastic modelling approaches** in energy storage investments (Ringkjøb et al., 2020; Seljom & Tomasgard, 2015)
- Role of **timeslices number and selection approaches** in energy storage deployment (with contributions from Paul Doods, Evangelos Panos, and Hiroshi Hamasaki)

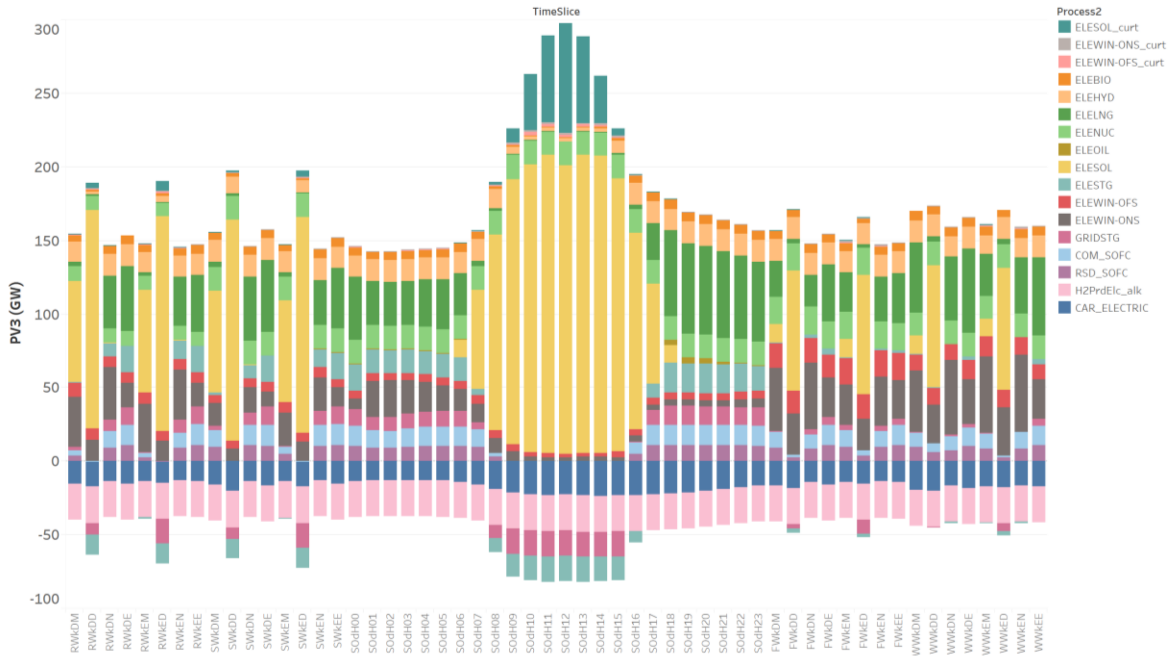

Figure 2: Asymmetric timeslices to capture flexibility and storage needs in TIMES (Hamasaki & Kanudia, 2019)

The second presentation (delivered by E. Panos on 03.02.2021) focused on the key modelling features of energy storage technologies with the TIMES framework, triggering a more in-depth technical discussion on how the different aspects of the technology are represented in the system. This presentation is also attached to this report in the file **ETSAP_TIMES_ST2_20210203.pdf** (Panos et al., 2021).

It discussed the main storage equations and provided an overview of the input parameters used to represent energy storage technologies in the model. Of particular interest to the Task 32 members was modelling the temporal resolution via the timeslice tree, maintaining the chronology using representative days, and linearising technical storage constraints, such as the degradation feature included in TIMES.

An overview of the plurality of technologies represented in the TIMES models operated by the different ETSAP members was also given, demonstrating the framework's strength in representing various types and scales of storage technologies (Figure 3).

Swiss TIMES	TIMES_PT	TIMES NATEM	JRC EU TIMES	UK TIMES
Electricity Storage	**Electricity Storage**	**Electricity Storage**	**Electricity Storage**	**Electricity Storage**
Hydro pump storage (new)	Hydro pump storage (new)	Hydro pump storage (new)	Diabatic Compressed Air Energy Storage	Pump hydro storage (8 hours)
Compressed Air Stora (adiabatic)	Battery storage (Lead-acid) High voltage	Compressed Air Storage (adiabatic)	Adiabatic Compressed Air Energy Storage	Pump hydro storage (24 hours)
Battery storage (Li-Ion NMC) high voltage	Battery storage (Li-ion) High voltage	Flywheel	Pump and Hydro Storage	Compressed Air Energy Storage.Converter.CAES
Battery storage (Li-Ion NMC) medium voltage	Battery storage (NaS) High voltage	Super Capcitor	Lead-acid batteries Utility scale	Compressed Air Energy Storage.CAES.
Battery storage (Li-Ion NMC) industry sector	Battery storage (Lead-acid) Buildings sector	Battery storage (Li-Ion) Utility Scale	Lithium-ion batteries Utility scale	Compressed Air Energy Storage.Turbine.CAES.
Battery storage (Li-Ion NMC) services sector	Battery storage (Li-ion) Buildings sector	Battery storage (Li-Ion) Small Scale	Sodium-sulphur batteries Utility scale	Advanced Adiabatic Compressed Air Energy Storage.CAES.8 Hour storage.
Battery storage (Li-Ion NMC) residential secto	Battery storage (NaNiCl ZEBRA) Buildings sector	Battery Storage (Vanadium Redox-flow)	Lead-acid batteries Residential	Advanced Adiabatic Compressed Air Energy Storage.CAES.24 Hour storage.
On-board car battery (small size cars)		Battery Storage (Lead-acid)	Lithium-ion batteries Residential	Battery.Sodium Sulphur.
On-board car battery (medium size cars)		Battery Storage (Sodium Sulfur)	ZEBRA batteries Residential	Battery.Lead Acid.
On-board car battery (large size cars)		Battery storage (Li-Ion) Residential	Lead-acid batteries Commercial	Battery.Redox Flow.4 Hour storage.
On-board car battery (SUV cars)		Battery storage (Li-Ion) Commercial	Lithium-ion batteries Commercial	Battery.Redox Flow.24 Hour storage.
On-board buses batte (small size buses)		**Thermal Storage**	ZEBRA batteries Commercial	Battery.Lithium Ion.
On-board buses batte (medium size buses)		Thermal Air circuit Residential Room Unit	Transport Batteries (already embedded within the Electric/Hybrid vehicles)	Liquid Air Energy Storage (LAES)
On-board buses batte (large size buses)		Thermal Air circuit Residential Home Unit	**Thermal storage**	**Thermal storage**
On-board buses battery (very large size buses)			Large Water Tanks	Large Water Tanks
On-board light duty vehicles battery			Underground Thermal Energy Storage	Underground Thermal Energy Storage
On-board heavy trucks battery			Large Water Tanks (cooling)	Pumped Heat Electricity Storage
Thermal Storage			Underground Thermal Energy Storage (cooling)	Hydrogen storage salt cavern
TCS storage - Industry			Hydrogen storage (only Tank)	Hydrogen storage (only Tank)
PCM storage - Services				
Water tank - Buildings				
Large scale district heating storage				
Liquid fuels storage (diesel, gasoline)				
Hydrogen storage in vessels				

Figure 3: Example of storage technologies represented in different TIMES models; the list is not exhaustive (Panos et al., 2021)

2.2 Joint workshop between ETSAP and ES TCP Task 32

A steppingstone in the collaboration between ETSAP and ES TCP Task 32 was to bridge the communication gap between technology experts and energy systems modellers and help them understand the challenges of representing storage technology in large-scale energy systems modelling frameworks. For this purpose, a designated joint workshop was held on 9.9.2021, which led to many fruitful discussions and furthered the understanding on the developer side.

The workshop brought together 16 colleagues from ETSAP and 13 colleagues from ES TCP Task 32 (see also the list of the workshop participants attached to this report file: **ETSAP_Task32_Participants_overview.pdf**). The workshop identified the main topics that the ETSAP teams would like to understand better regarding the storage technology and the main issues concerned the technology experts related to how accurately these technologies are represented in large-scale frameworks and how the simulation models being developed by them can be utilised or integrated into TIMES.

Upcoming workshop with ETSAP and TCP Energy Storage Task 32

Date: Thursday, Sept. 9th 2021, 4:30 pm (UTC+2) - Duration: 2,5 h

Place: Online (link will be communicated to the participants)

Group size: 15 from ETSAP + 15 from TCP Energy Storage Task 32 (not more than 30 people)

Registration: Doodle poll

Agenda

- 5 min short welcome
- 20 min presentation of ETSAP and TIMES modelling framework
- 20 min presentation of TCP Energy Storage Task 32
- 30-minute break out sessions (ca. 8) with 3-4 persons in each group (aim; socializing) -> in two rounds (heats) à 7 groups
- 45 min break out sessions A-D
  - Break out sessions A & B deal with the Thermal Storage
  - Break out sessions C & D deal with the Electrical Storage
  - The break-out sessions A & C discuss the exchanges from ETSAP/TIMES to Task 32 models and applications
  - The break-out sessions B & D discuss the exchanges from Task 32 models to ETSAP/TIMES
- 20 min oral presentations with the key discussion points from the breakout sessions A-D (each 5 min)
- 10 min follow up, identification of collaborations for the next workshop, and thank you

Figure 4: Agenda of the joint workshop between ETSAP and ES TCP Task 32.

The workshop agenda is shown in Figure 4 and featured two keynote presentations of ETSAP (delivered by G. Giannakidis) and ES TCP Task 32 (delivered by C. Doetsch), followed by breakout sessions on topics related to energy storage modelling and applications (see also the keynote presentations attached to the report **Introduction_ETSAP-TIMES.pdf** and **Introduction_Open_Sesame.pdf**)

The following subsection summarises the main topics discussed by the ETSAP teams, the topics relevant to the ES TCP Task 32 technology experts, and the main takeaways of the discussion.

2.2.1 Topics of interest in ETSAP related to energy storage modelling

The following topics were of particular interest among the participants from ETSAP, demonstrating the need for further discussions with technology experts around storage modelling:

a) Gain sufficient knowledge and data about the characterisation of energy storage technology, including important parameters to be considered in TIMES.
b) Get a better understanding of different aspects and issues related to storage modelling in long-term energy systems models and develop best practices in storage modelling in TIMES.
c) Improve the representation of variable renewables in TIMES models, especially in the context of consecutive days of low RE supply.
d) Establish a long-term collaboration with the energy storage technology experts in Task 32.

All ETSAP members who participated in the workshop recommended that the above topics be further elaborated in the context of additional workshops within ETSAP, with possible participation from colleagues from ES TCP Task 32.

2.2.2 Topics of interest in Task 32 related to energy storage modelling

From the side of ES TCP Task 32 colleagues, the main interest was in:

a) Get an overview of the current approaches and level of detail in energy storage representation in large-scale energy systems models.
b) Establish and maintain collaboration between technology experts and the energy systems modelling community.
c) Get a better understanding of the features, capabilities, applications, and limitations of the TIMES framework with a focus on energy storage technology.
d) Get an insight into the different needs and requirements of energy storage in different modelling applications and learn how large-scale energy systems integrate storage technology parameters and technical constraints.
e) Gain general knowledge on the TIMES modelling framework and its application in assessing energy flexibility projects, as well as how energy system modelling on different levels can be combined and which synergies can be used.

2.2.3 Summary of the discussions from the workshop

2.2.3.1 Discussions on what ES TCP Task 32 can provide to ETSAP

These discussions focused on two main questions:

- Which storage technologies are modelled in TIMES and how?
- How could collaboration with ES TCP Task 32 improve TIMES?

The discussion highlighted that TIMES models include a variety of storage technologies beyond the ones assessed in ES TCP Task 32, albeit representing them with linear constraints (L1 modelling in the terminology of the ES TCP Task 32). At the same time, the flexibility of developing TIMES models not only at national scales but also at district scales or even building scales was highlighted.

The following were identified as potential topics for which the ETSAP community can benefit from the storage technology expertise in ES TCP Task 32:

a) Use the detailed storage models developed in ES TCP Task 32 to validate or improve the TIMES models or even to couple TIMES with the detailed energy storage models of ES TCP Task 32.
b) Identify how to parametrise the TIMES model for the different energy storage technologies and, if possible, get these parameters from the energy technology experts of Task 32 (e.g., C-rates, efficiency, cycle life, etc.).
c) Identify suitable ways to deal with the aggregation in technology (e.g., multiple individual storage devices often in TIMES are bundled into a single process) and in time (e.g., how many timeslices are suitable for modelling the different storage technologies).
d) Identify operational constraints in storage technologies which can be entered into TIMES models. An important one is battery degradation, which is used to assess the reliability of battery operation in supporting transport electrification.

2.2.3.2 Discussions on what ETSAP can provide to ES TCP Task 32

This session focused on two main questions:

- Which technologies not represented in ES TCP Task 32 can come from ETSAP?
- How could collaboration with ETSAP improve the models in ES TCP Task 32?

The discussion identified that ES TCP Task 32 covered most energy storage technologies in TIMES models. However, the TIMES models also include storage options that were not covered by ES TCP Task 32 and for which technical and economic data are available from the different ETSAP teams:

- Hydrogen storage in tanks or underground
- Small-scale battery storage used in electric vehicles

In general, the experts from the ES TCP Task 32 were interested in getting the following insights from ETSAP:

- Possibility to jointly approach industry collaborators working, e.g. on batteries.
- Identify whether today's battery designs are conservative (or over-engineered) for the future energy system's needs.
- Assess the potential of second-life batteries, especially for electric vehicles.
- Get validated datasets from ETSAP related to renewable energy load profile, power system demand data, electricity prices, etc.

2.2.4 Key takeaways from the workshop

The workshop confirmed the well-acknowledged also in the past **need of the ETSAP community to exchange more often with technology experts**. This exchange is not only for parametrising the **representation of the different technologies** in TIMES but also for **validating TIMES results** with more detailed technology simulation models, including the possibility of **coupling TIMES** with these models. Regarding the energy storage technologies per se, the TIMES community seeks a better understanding of these technologies and ways to improve their representation in the model by integrating also improved model mechanisms capturing technologies' **operational constraints** (e.g., battery degradation and cycle-lifetime).

Technology experts are interested in learning **how technologies play a role in the future** energy system. For them, it is important to know whether the current technology designs are sufficient to meet the needs of a net-zero energy system regarding technology operation and reliability or to identify what additional improvements are needed. An important factor in achieving this objective is **closer collaboration with industry**. According to the technology experts, ETSAP should also be pursued more actively to ensure that the TIMES models stay up to date.

2.3 Contribution of TIMES to the ES TCP Task 32 final report

The ES TCP Task 32 final report also includes the TIMES modelling framework. It contributes to Subtask 2 (ST-2) of ES TCP Task 32 as an L1 energy systems model. It also contributes to Subtask 3 (ST-3) with selected applications (see section 2.1) for the deployment and role of energy storage technology in low-carbon energy systems. ES TCP Task 32 outcomes relevant to storage modelling

3. Storage Datasets and Models from ES TCP Task 32

3.1 Datasets collected in ES TCP Task 32

Subtask 1 (ST-1) of ES TCP Task 32 offered demonstration datasets for the storage models created in Subtask 2 (ST-2). Additionally, ST-1 provided information about openly available datasets or data models that could be utilised to apply the storage models in various regions worldwide. The data are openly accessible via the Open Energy Platform (OEP, https://openenergy-platform.org/). The OEP is a web interface that provides access to energy system modelling-related data such as power renewable generation potentials, power plant information and electricity and heat demand time series. It has a comprehensive and flexible metadata format to ensure all datasets are documented in compliance with open science standards.

A list of the datasets collected by the ES TCP Task 32 are provided in **Appendix 6.1** of this report. These include time series for different regions and countries, such as:

- Renewable energy sources profiles
- Electricity and heat load profiles
- Real-time storage operation profiles
- Electricity transmission grid topology and lines characterisation
- Electricity and heat generation profiles by source
- Metered data from real-cases electricity and thermal storage operation
- Technical characteristics of real-world electricity and thermal storage projects

Because these datasets do not include efficiency, lifetime, OPEX and CAPEX of energy storage, we also provide recent estimations for selected technologies. These are given in **Appendix 6.2** and include the following storage technologies:

- Batteries: Li-Ion, Lead-Acid, Vanadium Redox Flow
- Pump Hydrostorage
- Compressed Air Storage
- Hydrogen storage for gaseous and liquid H2, metal hydrides and LOHC
- Therma energy storage includes sensible, latent, phase change materials, and thermochemical and mechanical storage.

For electricity and hydrogen storage, we are based on (Bauer et al., 2022), and their techno-economic characterisation is summarised in Table 5 for electricity storage technologies and Table 6 for hydrogen storage technologies in Appendix 6.2. The technology costs and characterisation estimates for thermal storage technologies are from the IRENA technology innovation outlook (Boshell et al., 2020) and are summarised in Table 7 in Appendix 6.2.

3.2 Models developed in ES TCP Task 32

The following briefly overviews the developed simulation and optimisation energy storage models in ES TCP Task 32. **Appendix 6.3** of the current report provides more details about the models and references to their documentation.

The models developed in ES TCP Task 32 are non-linear. When their equations are linearised, this is accomplished with piece-wise techniques (which is mixed integer programming) or Taylor series expansion. Therefore, they cannot be directly embedded into the TIMES modelling framework. However, features of these models might be integrated into TIMES in future work, but only an approximation of these features can be implemented to maintain TIMES's linear property.

All models are available for downloading (code or documentation) via the Task 32 website (soon: https://iea-es.org/task-32/storage-models/)

3.2.1 Electricity storage models

The **compressed air energy storage and pumped hydro storage models** are based on a "reservoir model" approach, which describes a storage system as a charging unit, an energy reservoir, and a discharging unit. The units are connected via charging and discharging efficiencies. A toolchain was developed to consistently parametrise these models based on measured data or detailed dynamic simulation models.

The **Redox Flow Battery Model** is a simulation tool composed of a transient, two-dimensional model based on conservation principles (mass, momentum, and charge), incorporating the transport of the charged species and water. This transport model is combined with a kinetic model to simulate the performance of the all-vanadium RFB.

Four different models for **Li-Ion batteries** have been developed. The first is an online tool (named SoXery) that evaluates the ageing of a battery, given the usage conditions. The tool is based on a semi-empirical model. It takes power and temperature profiles of the battery from the user and the cell's chemistry to calculate the ageing the cell will undergo over a certain period. The output from the tool includes the calendar and cycle ageing in the cell, the increase in the internal resistance of the cell, and an unfulfillment map, which shows whether the cell was able to adhere to the usage profile or not. The tool is intended to be used as a first approximation by users who want to know the most appropriate cell chemistry given a usage profile or for sizing their battery for a specific purpose.

The second Li-Ion model is a linearised physics-based model to improve the accuracy and feasibility of the lithium-ion battery energy storage system operation strategy. The proposed model for the battery operation is built using physics concepts, and it is computationally attractive from the optimisation framework perspective. The focus of the model is the short-term operation of the battery.

The third Li-Ion battery model can be separated into two distinct portions: the electrical model and the thermal model. The electrical model consists of an equivalent-circuit model, which is not meant to describe the construction of the cell; rather, it describes the cell's high-level behaviour. The various components used to build this model (resistors, capacitors, etc.) are not actually present in the cell but act as analogues for some internal processes. The thermal model for the battery is a physic-based model that assumes the primary heat generator in the cell can be attributed to Joule heating. The model uses Joule’s law to calculate the power generated due to resistance, which is proportional to heat flow from the resistor if it is assumed that all electrical losses in the resistor are converted into heat.

The fourth Li-Ion model is a machine learning model. It is a battery cell surrogate model for voltage estimation using deep learning methods. In this case, ‘surrogate’ refers to the fact that the model is intended to act as a complete black box model and does not include any true physics. The model was developed to estimate a cell's voltage at a given current, state of charge (SOC), and temperature operating condition.

The **Na-Ion Battery Model** is an integrated modelling framework for assessing the performance, costs, and environmental impacts of Lithium-Ion-Batteries (LIB) and Na-Ion-Batteries (NIB) cells. It consists of a physics-based pseudo-two-dimensional (P2D) battery cell model to assess the performance of battery cells subjected to varying discharge rates, a bottom-up battery cell cost model and a model to quantify the environmental impacts of battery cells based on life cycle assessment.

The following table provides an overview of the electrical models developed in Task 32.

Table 1: Overview of the electricity storage models developed in ES TCP Task 32

Technology	Model level	Model source	Scope	Input data	Output data	Programming Language	Simulation / Optimisation
Com-pressed-air energy storage (CAES)	L1	**FhG-UMSICHT** E.Schischke K. Wode M. Hadam	Adiabatic	Efficiency curve, storage size	Time series of input / output power	Python	Optimisation
Pumped hydro	L1	**FhG-UMSICHT** E.Schischke K. Wode M. Hadam	Separate machine trains, pump turbine	Efficiency curve, storage size	Time series of input / output power	Python	Optimisation

Technology	Model level	Model source	Scope	Input data	Output data	Programming Language	Simulation / Optimisation
Redox Flow Battery		**NRC-KR(KIER)**	Vanadium RFB single and stack cell system	cell geometry, flow rate, power, current	Capacity current, voltage, time	COMSOL Multiphysics	Simulation
Li-ion Battery	L2	**ESReC (BFH+CSEM)** P. Caliandro C. Brivio	Li-ion battery performance model with degradation	Battery size, power & energy use profiles, temperature profiles, chemistry type (NMC, LFP, LTO)	Energy efficiency, degradation rate	Python	Simulation
Li-ion Battery	L2	**Ucalga-ry + NRC** A.Vykhodtsev	Linearised battery model	Battery size and parameters of a lithium-ion cell	Dispatching profile of the battery	Julia	Optimisation
Li-ion Battery	L2	**NRC** A. Crain, D. Jang	Equivalent Circuit Model	Battery cell technical parameters and material properties	Discharge and charge performance	Modelica	Simulation
Li-ion Battery	L2	**NRC** A. Crain, D. Jang	Surrogate battery model	Current load, state of charge and temperature	Cell voltage time series	Julia & Python	Simulation
Li-ion Battery	L2	**NRC** A. Crain, D. Jang	NARX State-of-Charge Predictor	Active power, state of charge	State of charge prediction at the next time step	Julia & Python	Simulation
Li ion Battery	L2	**PSI** S. Schneider E. Panos	P2D battery cell model coupled with LCA	Cell technical data, geometric data and material data	Charing and discharging profiles, manufacturing costs and LCA environmental impacts	MATLAB & Python	Simulation & cost optimisation
Na-ion Battery	L2	**PSI** S. Schneider E. Panos	P2D battery cell model coupled with LCA	Cell technical data, geometric data and material data	Charing and discharging profiles, manufacturing costs and LCA environmental impacts	MATLAB & Python	Simulation & cost optimisation

3.2.2 Thermal storage models

The Subtask 2 Thermal group focused on developing and applying methods for assessing the performance of heat-to-heat storage devices. These technologies are less standardised than electric-to-electric storage devices and are often custom-designed and integrated within buildings and other end-use applications. Various heat-to-heat storage technologies exist, each suited to different temperature ranges. High-temperature applications (>500°C) can be used in concentrated solar thermal power plants, while other technologies at lower temperatures are used in cool thermal energy storage for industrial refrigeration. Heat-to-heat energy storage is most commonly used in building and community heating systems and for domestic hot water heating, which require moderate temperatures (40 to 80°C).

Three categories of materials can store thermal energy: sensible, latent, and thermochemical. **Sensible materials** increase their internal energy and temperature without undergoing a phase or chemical change. Common materials used for sensible storage are water, soil, rocks, and bricks due to their high specific heat capacity and density. **Latent materials** undergo phase changes during charging and discharging (e.g., solid-to-liquid) and thus take advantage of the relatively large change in internal energy associated with the physical state change. They offer advantages such as higher energy storage density and lower self-discharge. However, issues like cost, material stability, and low thermal conductivity have limited their widespread use. The third category, **thermochemical storage**, relies upon chemical reactions or sorption phenomena. When charging, the energy input serves to excite a reversible chemical reaction, that is, some change in the molecular arrangement of the material. Often, this takes the form of the adsorption of a gas within a solid. There is much active research on thermochemical storage, but applications for heat-to-heat applications are relatively few to date. The interested reader is referred to (Tatsidjodoung et al., 2013), who offer a thorough review of heat-to-heat storage options for building applications. A similar review pertaining to the seasonal storage of solar thermal energy, as well as an overview of modelling methods for sensible storage, is provided by (Pinel et al., 2011).

The Subtask 2 Thermal group participants were researching a wide range of heat-to-heat energy storage technologies. These included **sensible pit and water tank storage** for community-scale applications, **water tank and wet sand storage** for the seasonal storage of solar thermal energy at the single-building scale, **sensible storage within the structure of the building**, and **aquifer thermal energy storage** for community-scale applications. All of these are sensible storage options. Some participants were exploring phase change technologies and sorption-type thermochemical technologies, but this work was less developed within the context of Task 32.

4. MODELLING STORAGE IN TIMES: PRACTICES AND CHALLENGES

4.1 Practices used for storage modelling in TIMES

TIMES offers sophisticated storage modelling with many features and functionalities to capture the technology's complexity as accurately as possible within the boundaries of a linear programming framework.

4.1.1 Types of storage in TIMES and examples

A storage technology in TIMES is usually defined by most users as operating only at one level of the timeslice tree (**STG** type) or across multiple levels of the timeslice tree (**STS** type). More seldom in TIMES models is the specification of storage to operate across periods (**STK** type). The STK type can also be combined with STS and have an interperiod storage to operate across the timeslice tree's levels. In addition, storage technology can also be a demand technology by adding the corresponding modifier (DMD) in its definition.

Below some examples of practices followed in ETSAP are presented for different types of storage systems:

- **Battery**: usually, a battery is modelled as STG at the DAYNITE level, although batteries with large energy capacity can be modelled as STS at the WEEKLY level (which also implies operation at the DAYNITE level). However, batteries with small capacities in terms of energy but with high output power are modelled at the DAYNITE level as these batteries aim to provide a fast balancing relief to the grid.
- **Pump hydro storage** and **compress air storage** are usually modelled as STS at the WEEKLY level. Still, depending on the definition of the timeslice tree, a DAYNITE-only operation of pump hydro storage can also be considered (i.e., STG type).
- **Hydrogen storage** is more suitable for modelling as STS operating at the SEASONAL level (which also implies operation at WEEKLY and DAYNITE levels).
- **Thermal storage**: On-site units usually operate at the DAYNITE level (STG), while larger units at the district level should be modelled as STS.
- **Stockpiling, including waste disposal and hydropower with dams**: These can be modelled as inter-period storage (STK), and, in the case of hydropower units with dams, they can also be modelled as STK+STS storage, if desired by the TIMES user.

When defining a storage process, the commodity is usually the same on the input and output sides. However, this can lead to a situation where the storage is bypassed in the same time slice and period, resulting in arbitrarily large input or output flows. To avoid this, the commodity entering or leaving storage should be defined as an input or output flow. The user can choose this.

4.1.2 Storage related variables

Four main variables are related to storage: **VAR_ACT** represents the amount of stored energy, VAR_NCAP represents the capacity (expressed in power or energy terms) of the storage technology, and VAR_SIN/VAR_SOUT represents the charging and discharging flows.

It should be noted that the VAR_SIN/SOUT variables cannot be referred to via UC_FLO in the user constraints, and auxiliary flows should be attached to them for this purpose.

4.1.3 Commonly used storage technical parameters

TIMES offers a large set of parameters to characterise the storage technology. The most used ones are listed below, and we direct the reader to the TIMES Documentation Part II for correctly using these parameters. In the following, r is a region, p is the storage process, c is the commodity entering or leaving the storage, s is the timeslice, tsvl is the timeslice tree level, and bd is the type of the bound (LOwer, UPper, FiXed):

- **STG_CHRG**(r,y,p,s): exogenous charging of storage that can be used, for example, to model water inflow in a hydrostorage.

- **STG_EFF**(r,y,p): roundtrip efficiency.

- **STG_LOSS**(r,y,p,s): annual storage losses, i.e., self-discharge as a fraction of the average yearly amount stored.

- **STGIN_BND**(r,y,p,c,s,bd) and **STGOUT_BND**(r,y,p,c,s,bd): bound (bd=LO, UP, FX) on the charging (STGIN_BND) or discharging (STGOUT_BND) commodity.

4.1.4 Advanced storage technical parameters

Besides the common parameters listed above, TIMES offers a range of more advanced storage parameters, which are summarised below:

- **STG_MAXCYC**(r, y, p): limit for the storage cycling as a maximum number of charging cycles allowed. The definition of the cycle is charging followed by discharging, independent of the depth of discharge.

- **STG_SIFT**(r,y,p,c,s): when enabled, the storage is a load-shifting mechanism, and the parameter defines the maximum fraction of shift load c in proportion to demand at the DAYNITE level (and the level above, if desired) in timeslice s. Combined with the STGIN_BND/STGOUT_BND, it can prevent the shifting. Combined with ACT_TIME, it can define the load shift window, e.g., 5h in advance (UP) or delay (LO). Combined with ACT_CSTRMP, discomfort costs can be defined for shifting the demand by 1h forward (UP) or backward (LO).

- **NCAP_AFC**(r,y,p,cg,tslvl): defines availability factors for the process activity (amount stored), process output flow or process input flow, or any combination of these. When it is imposed on the output or input flow (if the same, the input flow should be defined with the special keyword “NRG” in the parameter), it can impose maximum charging and discharging rates (C-rates).The NCAP_AFC expresses the ratio of the energy capacity to the nominal maximum energy output during one cycle of the storage timeslice level (i.e. 1 day for DAYNITE, 1 week for WEEKLY, 1 year for SEASON): for example, if the energy capacity represents an 8h of storage, NCAP_AFC(ACT) = 8/24/STG_EFF.

- **BS_STIME**(r,t,p,b,bd): Defines the times (in hours) for reserve provision from storage process p for reserve b in region r. When bd='LO' it refers to the time required for a storage process to ramp up to provide reserve b, e.g. for FCR-type reserve can be 0.01, for aFRR-type of reserve can be 0.13, etc.. When bd='UP' it corresponds to the duration of the provision of reserve b from a storage process, also including the time to ramp up. E.g. the duration of a aFRR-type of reserve can be 7.0 min, and if we assume that the process needs 0.13 min to ramp up, then the parameter BS_STIME ('UP') should be set to 7.13/60 hours.

Additional parameters for defining the storage processes, for example, costs or parameters for auxiliary flows, are provided in the TIMES Documentation Part II. It should be noted that ramping rates, ramping/startup/shutdown costs, minimum online/offline times, minimum stable operating levels, part load efficiency losses and other dispatching parameters do not apply to storage. A possible extension of TIMES might consider including the ramping rates and costs, provided that the capacity of the storage process is expressed in power and not in energy terms (i.e., the NCAP_AFC on ACTivity is used).

4.2 Modelling of battery degradation in TIMES

In the Ancillary Services Extension of TIMES, the modelling of storage degradation is introduced, which is now included in the vanilla version of the framework as a standard via the **STG_MAXCYC** parameter. The purpose of this parameter is to approximate the impact of storage degradation on investment decisions by assuming a targeted number of cycles per year.

For example, if we assume that the calendar lifetime of the storage is 10 years and the cycle life is 4500 cycles, this results in 450 cycles per year on average if both the calendar and the cycle lives are to be respected. If the number of cycles in a year exceeds the annual targeted number of cycles, in our example is 450 cycles, then this means that implicitly a storage replacement has happened – please recall that the storage process in TIMES will remain in place for its whole calendar life, so if the cycles in a year are above the targeted number of cycles the storage process cannot operate for its entire calendar life because its cycle life does not permit this anymore without a replacement.

In the case when the cycle life of the storage process is reached, TIMES calculates the required replacement capacity to continue operating the storage for the rest of its technical lifetime. The cost of the replacement capacity enters the objective function.

4.3 A new extension in TIMES for storage dispatching

In (Kotzur et al., 2018), an alternative approach for linking typical representative days (such as seasons) was presented, compared to what is used in TIMES. The formulation in (Kotzur et al., 2018) considers that the variation in the total storage level SoC can occur around the seasonal state (VAR_ACT at the beginning of the season), both upwards and downwards, as long as the total value of SoC remains non-negative.

In contrast, in TIMES, the total storage level SoC is assumed to be greater than or equal to the corresponding seasonal state. This entails some inflexibility in the dispatching of storage.

A new extension of TIMES has been implemented (Lehtilä, 2022), which follows the principle of (Kotzur et al., 2018). The new extension allows the DAYNITE variation of the storage level SoC to take place around (and not above anymore) the intra-seasonal state of charge.

All the implementation details are described in (Lehtilä, 2022), but whether this assumption from (Kotzur et al., 2018) is reasonable is open. Therefore, the ETSAP teams are invited to test the extension and provide feedback on whether it is reasonable or not to assume that the DAYNITE variation may occur both above and below the seasonal state of charge in TIMES and not always above the seasonal state of charge as it is currently.

The new extension can be enabled by setting it in the .RUN file:

```
$SET STSFLX YES
```

For more details, please see (Lehtilä, 2022)

4.4 A SubRES template for modelling storage in TIMES

Attached to the report is a SubRES template created by Antti Lehtilä that demonstrates the use of different storage parameters in modelling the various types of storage technologies. The SubRES is included in the file **SubRES_Storage-v2.zip.**

It contains comprehensive examples of modelling storage options such as:

- Concentrating solar
- Hydropower with pondage
- Hydropower with a large reservoir
- Pumped hydro
- CAES
- Utility scale batteries
- Small scale batteries
- Electric vehicle storage
- District heating storage
- Hydrogen storage
- Coal stockpile storage

In addition, the modelling of demand response load shifting is demonstrated through a storage process.

The file demonstrates the use of all storage parameters mentioned in sections 4.1.3 and 4.1.4. The provided initialisation of the storage parameters is documented in the file as a comment/note in the corresponding cell.

We hope the SubRES will help many users model the storage technology correctly in TIMES.

4.5 Challenges in modelling storages in TIMES models

There are several characteristics of long-term energy optimization models, ESOMs, including TIMES models, that can influence the model results on investments and use of energy storages in conducted energy system analysis. Below, some relevant challenges are identified with suggestions on how to overcome these.

A first issue is the **spatial resolution**. In TIMES models that covers larger regions, the modelled storages often represent an aggregation of storage options in that region. If the modelled storages are not constrained, this can overestimate the value of this storage.

For example, when analysing storages in buildings, as stationary batteries, the model can wrongly estimate how much of the total demand that can be shifted, since it appears as a "large building" instead of many smaller buildings. How much of the demand that can be shifted, depends on the relationship between the storage capacity and demand in each of the buildings in the region.

Another example is when hydropower reservoirs in a region is modelled as one single storage process, but the region has in real life several hydro reservoirs. Unless the flexibility of the reservoir is constrained, this can give a too flexible representation of the hydropower production. This is because an aggregation does not consider local conditions of each of the power plants. It can for example be that at some locations, the production capacity is constrained due to limited reservoir capacity or due to restrictions in ramping rates of the reservoir.

Therefore, to provide trustworthy results of energy storages, it can be important to constrain the storages, and to critically evaluate the results in light of the spatial aggregation. A consequence, though, is that including constraints on storage processes increases the computational complexity. To avoid this, it is an option to replace the use of energy storages with flexible process technologies. For example, flexible hydropower does not have to be modelled by using a storage process, but can be represented by using a flexible process, with e.g., upper and lower bounds. This can contribute to lower the computational time of the analysis.

A second issue is that most TIMES models apply **perfect foresight**. This implies that the model assumes that there is no prediction error in production and demand, that again can underestimate the need for flexibility, including energy storages. For example, the use of storages can be a suitable solution to use energy when the production is higher than expected, and to supply energy when the production is lower than expected. One method to account for prediction errors and the need for back-up capacity is to apply the Ancillary Services Extension of TIMES. This increases the computational complexity of the analysis but can be relevant to include when flexibility and energy storages plays an important role in the analysis.

A third issue is the representation of the **weather dependent renewables and demand** in TIMES models. This is because the weather that influences the production and demand differs within a day and between seasons and years, that again defines the need for flexibility and energy storages.

There are several options to capture weather dependent renewables and demand.

- A first approach is to <u>increase the temporal resolution</u> of the model that is within a computational tolerance. For this approach, it can be beneficial to develop the TIMES model to have a flexible time-slice option. Meaning, the TIMES models is designed to be easily run with different time-slices. This can be done by using hourly time-slice dependent parameters as an input, that is aggregated based on the desired temporal resolution. Such a methodology enables the use of a lower temporal resolution (and lower solution time) when developing and testing the model, and to use a finer temporal resolution in the final analysis. Also, it allows for analysing how a different temporal resolution effects the model results, including investments and operation of energy storages.
- A second approach is to use statistical methods to <u>select representative days</u> from an hourly time series of a year as model input, as the ETSAP time-slice tool. A common feature of most of these methods is that they only consider the input data and not the corresponding results, when selecting representative days. This can thus give biases related to the weighing of various weather dependent parameters.
- A third approach is to use the <u>stochastic modelling</u> options that is included in the TIMES code. Stochastic modelling is a mathematical method to better consider uncertainty and to value flexibility (including energy storages) in optimization models. Compared to using a deterministic approach, that use only one realisation of the weather-dependent parameters per time-slice, a stochastic modelling approach inputs a discrete distribution of the weather-dependent parameters. This allows for investments, including in energy storages, that considers for that the weather-dependent parameters can have different realisations. Further, such an approach gives operation of the storages that are made for different realisations of the weather. Note that a stochastic modelling approach increases the computational complexity and requires a generation of consistent stochastic scenarios.

5. OUTLOOK AND CONCLUSIONS

Within the ES TCP Task 32, a variety of datasets useful for modelling energy storage systems were collected, and a significant number of energy storage models were developed, including electrical energy storage systems and thermal energy storage systems. The datasets are now/soon available on the Open Energy Platform (https://openenergy-platform.org/), while the models are described in the ES TCP Task 32 report and are available now/soon via the Task 32 website (https://iea-es.org/task-32/storage-models/). The provided models are characterised by a classification system developed by Task 32 to assess the level of detail of the storage model easily. L1 models represent storage technologies with linear constraints, while L2 models include non-linear effects of storage operation and more detailed technology representation.

Most of the models developed in ES TCP Task 32 are non-linear. When their equations are linearised, this is accomplished with piece-wise techniques (which is mixed integer programming) or Taylor series expansion. Therefore, they cannot be directly embedded into the TIMES modelling framework. However, features of these models might be integrated into TIMES in future work, but only an approximation of these features can be implemented to maintain TIMES's linear property.

An important outcome of the collaboration between ETSAP and Task 32 is the need for improved awareness of the communication challenges that developers of different models' face. This collaboration originally aimed at breaching the gap between the understanding of energy storage systems for large-scale energy system model developers and very detailed- and technology-orientated developers of simulation models. While the joint workshop led to fruitful discussions and furthered the understanding of technology on the developer side, the communication barriers between technology experts focusing on simulation models and developers of energy systems models were not entirely lifted.

There is an increased need for continued discussion between technology experts and the energy systems analysis and modelling community. This first step regarding storage technology identified many common areas and topics that need to be elaborated on between the two communities in future workshops and collaborations.

6. APPENDIX

6.1 Energy storage related datasets from ES TCP Task 32

Input data for energy storage models can be electrical or thermal generation from an individual variable renewable energy resource in an island supply system or from several energy resources in a larger energy system. It can also be economic parameters such as time-based pricing data for electrical or thermal energy or aggregated load profiles at different scales ranging from an individual plant or project to a national region.

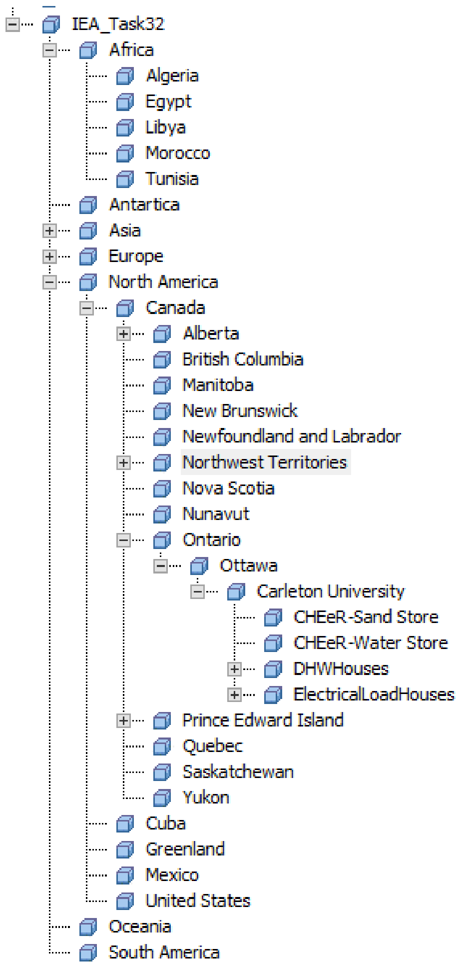

Figure 5: Asset structure for data navigation in the NRC PI data system

ES TCP Task 32 intended to collect meaningful example data sets that could be used by models developed in Subtask 2 or by simulation platforms using various models in Subtask 3. The collected datasets on load profiles are at different spatial scales. Canada's National Research Council (NRC) served to collect and host the various data sets provided to the Task 32 project using its PI System data historian platform. An asset structure for navigating into the data was created as well, which is shown in Figure 5.

ES Task 32 collected two types of datasets: datasets generated outside of Task 32 and datasets generated within Task 32.

The collected data will be published on the Open Energy Platform (OEP, https://openenergy-platform.org /). The OEP is a web interface that provides access to a database for energy system modelling-related data such as power renewable generation potentials, power plant information, and electricity and heat demand time series. It has a comprehensive but flexible metadata format to ensure documentation of all datasets that are machine-readable and compliant with open science standards.

Table 2: list of datasets collected in ES TCP Task 32 that provide temporal renewable power generation and power demand profiles and were generated outside ES TCP Task 32

			Spatial		**Temporal**				**Energy demand**		
Dataset	**Institution**	**Link**	**Extent**	**Resolution**	**Extent**	**Resolution**	**Technologies**	**Data source**	**Electricity**	**Heat**	**Cooling**
ENTSO-E + derivatives (e.g. OPSD)	ENTSO-E	[1]	Europe	country / control areas / bidding zones	2006 - today	15 min - 1 h	PV, wind	ENTSO-E	+	-	-
EMHIRES	JRC	[2]	Europe	NUTS2 / countries / bidding zones	30 a (1986-2015)	1 h	PV, wind	ERA5, COSMO-REA6, thewindpower.net, MERRA	-	-	-
ENSPRESO	JRC	[3]	EU-28	NUTS2 / countries	40 a (2010-2050)	annual, year fractions	PV, wind, biomass, CSP	MERRA, GWA, METEOSAT	-	-	-
Global Atlas for Renewable Energy	IRENA	[4]	global	diverse	diverse	monthly / annual	PV, wind, marine, bioenergy, geothermal, hydropower	diverse	-	-	-
Global Wind Atlas	DTU	[5]	global	250 m	2008-2017	none (long term average)	wind	ERA5	-	-	-

[1] https://transparency.entsoe.eu/ and https://data.open-power-system-data.org/time_series/2020-10-06
[2] https://publications.jrc.ec.europa.eu/repository/handle/JRC105937 and https://data.jrc.ec.europa.eu/collection/id-0055
[3] https://doi.org/10.1016/j.esr.2019.100379 and https://publications.jrc.ec.europa.eu/repository/handle/JRC116900 and https://data.jrc.ec.europa.eu/collection/id-00138
[4] https://globalatlas.irena.org/workspace
[5] https://globalwindatlas.info/en

Table 3: Data models identified in ES TCP Task 32 providing temporal renewable power generation and demand profiles

			Spatial		Temporal				Energy demand		
Model	**Institution**	**Link**	**extent**	**resolution**	**extent**	**resolution**	**Technologies**	**Data source**	**Electricity**	**Heat**	**Cooling**
PyPSA Atlite	FIAS	[1]	global	31 km	40-150 a	1 h	wind, PV, solar thermal, hydro	ERA5, Sarah2, NCEP, EURO-CORDEX	-	+	-
reV	NREL	[2]	Americas, south and central Asia, south Africa	local - international, depending on the resource	Americas: 1998-2021 Europe: 2017-2019	15 min - 1 h	onshore wind, PV, CSP	NSRDB: National Solar Radiation Database, Wind Integration National Dataset Toolkit	-	-	-
Renewables Ninja	ETH/ICL	[3]	global	single location, country aggregated	32 a (PV) 37 a (wind)	1 h	PV, wind	SARAH, MERRA	-	-	-
Global Energy GIS	Chalmers University	[4]	global	country level / 31 km / (1km)	40 a	1 h	wind, PV, CSP	ERA5	+	-	-
RESKit	FZJ - IEK	[5]	global	single location	24 - 150 a	1 - 3 h	wind, PV	Cosmo-REA6, ERA5, EURO-CORDEX, MERRA	-	-	-
pyGreta	TU München	[6]					wind, PV, CSP	MERRA2			
ENTSO-E and derivatives (e.g. OPSD)	ENTSO-E	[7]	Europe	country / control area / bidding zone level	2006 - today	15 min - 1 h		ENTSO-E	+	-	-

[1] https://joss.theoj.org/papers/10.21105/joss.03294 and https://github.com/PyPSA/atlite
[2] https://www.nrel.gov/gis/renewable-energy-potential.html
[3] https://www.renewables.ninja/
[4] https://doi.org/10.1016/j.esr.2020.100606 and https://github.com/niclasmattsson/GlobalEnergyGIS
[5] https://doi.org/10.1016/j.energy.2019.06.052 and https://github.com/FZJ-IEK3-VSA/RESKit
[6] https://github.com/tum-ens/pyGRETA
[7] https://transparency.entsoe.eu/ and https://data.open-power-system-data.org/time_series/2020-10-06

Table 4: Datasets collected within the ES TCP Task 32

Data Provider	Type of data	Source of data	Geographical range	Geographical resolution	Temporal Range	Temporal resolution	Nr. of time series
UA[1]	Electric Load	Metering data	Province	Sub-station (48)	2011-01-01 12:00am - 2022-02-28 11:00pm	1 hour	1
UA	Wind Generation	Metering data	Site (16)	NA	2010-01-01 12:00am - 2021-12-31 11:00pm	1 hour	1
UA	PV generation	Metering data	Site (13)	NA	2010-01-01 12:00am - 2021-12-31 11:00pm	1 hour	1
UA	Energy Storage	Metering data	Site (3)	NA	2010-01-01 12:00am - 2021-12-31 11:00pm	1 hour	1
NTPC[2]	Electrical Load	Metering data	Community	NA	2018-01-01 12:00am - 2019-07-31 10:45pm	1 minute	38
NTPC	Diesel Generation	Metering data	Community	NA	2018-01-01 12:00am - 2019-07-31 10:45pm	1 minute	36
NTPC	PV Generation	Metering data	Community	NA	2018-01-01 12:00am - 2019-07-31 10:45pm	1 minute	15
NTPC	Energy Storage	Metering data	Community	NA	2018-01-01 12:00am - 2019-07-31 10:45pm	1 minute	30
DLR[3]	Electrical Load	Simulation data	Continent	Country (31)	2050-01-01 12:00am - 2050-12-31 11:00pm	1 hour	1
DLR	Thermal Load	Simulation data	Continent	Country (31)	2050-01-01 12:00am - 2050-12-31 11:00pm	1 hour	1
DLR	Wind Generation (offshore)	Simulation data	Continent	Country (31)	2050-01-01 12:00am - 2050-12-31 11:00pm	1 hour	1
DLR	Wind Generation (onshore)	Simulation data	Continent	Country (31)	2050-01-01 12:00am - 2050-12-31 11:00pm	1 hour	1
DLR	PV generation	Simulation data	Continent	Country (31)	2050-01-01 12:00am - 2050-12-31 11:00pm	1 hour	1
CU[4]	Flow rate	Demonstration data	Site	NA	2020-01-29 12:02am - 2021-04-27 11:57pm	5 minutes	11

CU	Heat transfer	Demonstration data	Site	NA	2020-01-29 12:02am - 2021-04-27 11:57pm	5 minutes	28
CU	Electrical Load	Demonstration data	Site (16)	NA	2011-06-29 11:00pm - 2012-06-28 10:59pm	1 minute	3
CU	Themal Load	Demonstration data	Site (12)	NA	2007-01-01 8:05am - 2008-01-01 8:00am	1 minute	1
KIER[5]	Energy Storage	Laboratory data	NA	NA	2021-03-15 3:15pm - 2021-03-15 7:03pm	30 seconds	3
WEIC[6]	Wind Generation	Metering data	District	NA	2021-04-30 5:00pm - 2021-12-30 4:00pm	5 seconds	13
WEIC	PV Generation	Metering data	District	NA	2021-04-30 5:00pm - 2021-12-30 4:00pm	5 seconds	25
WEIC	Energy Storage	Metering data	District	NA	2021-04-30 5:00pm - 2021-12-30 4:00pm	5 seconds	6
KU[7]	PV generation	Metering data	Site	NA	2016-09-01 12:00am - 2022-12-31 11:59pm	1 minute	6
KU	Energy Storage	Metering data	Site	NA	2017-11-01 12:00am - 2020-06-17 7:02pm	1 minute	11

6.2 Cost and characterisation for selected energy storage technologies

The tables below summarise the cost and characterisation for selected energy storage technologies, which were collected from data sources outside the ES TCP Task 32.

Table 5: Overview of electricity storage key characteristics (Bauer et al., 2022)

Technology	Attribute	2020	2035	2050
Battery Li Ion	TRL	9		
	Roundtrip efficiency (%)	85-95		
	Response time (sec)	1		
	Lifetime (years)	10 -15		
	Cycles at 80% depth of discharge	3500		
	Optimal depth of discharge (%)	80 – 93		
	Energy-to-Power ratio (large scale / small scale)	6/2		
	CAPEX EUR/kW (large scale/small scale)	160/1600	80/800	60/600
	CAPEX EUR/kWh	200	100	75
	OPEX EUR/kW/a (large scale / small scale)	0/10		
Battery Lead-Acid	TRL	9		
	Roundtrip efficiency (%)	70 – 80		
	Response time (sec)	1		
	Lifetime (years)	10		
	Cycles at 80% depth of discharge	900		
	Optimal depth of discharge (%)	50 – 60		
	Energy-to-Power ratio (large scale / small scale)	6/2		
	CAPEX EUR/kW (large scale/small scale)	400/1500		250/1000
	CAPEX EUR/kWh	500		100
	OPEX EUR/kW/a (large scale / small scale)	0/10		
Battery Vanadium Redox Flow	TRL	7		
	Roundtrip efficiency (%)	60 – 75		
	Response time (sec)	1		
	Lifetime (years)	20		
	Cycles at 80% depth of discharge	10000		
	Optimal depth of discharge (%)	50 – 60		
	Energy-to-Power ratio	6 - 8		
	CAPEX EUR/kW	1600		1000
	CAPEX EUR/kWh	800		300
	OPEX EUR/kW/a	40		
Compressed Air Energy Storage Adiabatic	TRL	5-6		
	Roundtrip efficiency (%)	70 – 85		
	Response time (min)	3 – 10 min		
	Lifetime (years)	20 – 60		
	Cycles at 80% depth of discharge	10000		
	Optimal depth of discharge (%)	n.a.		
	Energy-to-Power ratio	5 – 8		
	CAPEX EUR/kW	1200		1000
	CAPEX EUR/kWh	300		200
	OPEX (% of CAPEX)	2.5		
Pump hydro storage	TRL	9		
	Roundtrip efficiency (%)	70 – 85		
	Response time (sec)	FS	AS	Ternary
	Spinning-in-air to full load generation	5-70	60	20-40
	Shutdown to full load generation	65-120	90	65-90
	Spinning-in-air to full load	50-80	70	25-30

Technology	Attribute	2020	2035	2050
	Shutdown to full load	160-360	230	80-85
	Full load to full generation	90-220	280	25-60
	Full generation to full load	240-500	470	25-45
	Lifetime (years)	40– 120		
	Cycles at 80% depth of discharge	15000		
	Optimal depth of discharge (%)	n.a.		
	Energy-to-Power ratio	>8		
	CAPEX EUR/kW)	500 – 5000 (avg 2200)		
	CAPEX EUR/kWh	10 – 100		
	OPEX (% of CAPEX)	2 – 10		

Table 6: Overview table representing storage pressure levels, CAPEX, OPEX and lifetime of the considered hydrogen mediums (Bauer et al., 2022)

Storage	Gaseous	Liquefied	Caverns	Metal Hydrides	LOHC	Unit
Storage pressure	15-700	~1	45-300	~10-60	2-70	bar
CAPEX	220-2200	~330	1-3	1400-3600 (tank plus hydride material)	No data	CHF/kg H2 storage
OPEX	2%	2%	2%	No data	4%	% of CAPEX
Lifetime	20-25	20	30-50	25	25	years

Table 7: Key technical and cost attributes of selected thermal energy storage technologies (Boshell et al., 2020)

Type	Technology	Attribute	-	2020	2035	2050
Sensible[1]	WTTES	Range of capacities	kWh - 1 GWh			
		Range of power	kW- MW			
		Operating temperature	10 – 90 ºC			
		Round-trip efficiency	50 – 90%			
		Storage period	hh – mm			
		Energy density	15-80 kWh/m²			
		Lifetime (yrs or # of cycles)	15 – 40 yrs			
	UTES	Range of capacities	MWh - GWh			
		Range of power	MW - 100 MW			
		Operating temperature	5– 95 ºC			
		Round-trip efficiency	up to 90%			
		Storage period	ww - mm			
		Energy density	25-85 kWh/m²			
		Lifetime (yrs or # of cycles)	50 yrs			
	Solid state	Range of capacities	10 kWh - GWh			
		Range of power	kW - 100 MW			

[1] Sensible storage: tank thermal energy storage (TTES) using water as a storage medium (WTTES), solid-state thermal storage (e.g. ceramic bricks, rocks, concrete, packed beds), molten salts, underground thermal energy storage (UTES)

Type	Technology	Attribute	-	2020	2035	2050
		Operating temperature	-160 to 1300 °C			
		Round-trip efficiency	>90%			
		Storage period	hh – mm			
		Energy density	0.4-0.9 kWh/m^3			
		Lifetime (yrs or # of cycles)	>5000 cycles			
	Molten salts	Range of capacities	MWh - 5 GWh			
		Range of power	100 kW - 300 MW			
		Operating temperature	265 – 565 °C			
		Round-trip efficiency	>98%			
		Storage period	hh – dd			
		Energy density	70-200 kWh/m^2			
		Lifetime (yrs or # of cycles)	>20 yrs			
	All sensible TES	Cost ($/kWh)		25-30	<15	<12
		Efficiency roundtrip (%)		>90	>92	>95
Latent[1]	Ice storage	Range of capacities	kWh - 100 MWh			
		Range of power	kW - 10 MW			
		Operating temperature	-3 - 3 °C			
		Round-trip efficiency	>95%			
		Storage period	hh – dd			
		Energy density	92kWh/m^2			
		Lifetime (yrs or # of cycles)	>20 yrs			
	SZ PCM	Range of capacities	kWh - 100 MWh			
		Range of power	kW - 10 MW			
		Operating temperature	down to -114°C			
		Round-trip efficiency	>90%			
		Storage period	hh			
		Energy density	30-85kWh/m^2			
		Lifetime (yrs or # of cycles)	>20 yrs			
	LT PCM	Range of capacities	kWh - 100 MWh			
		Range of power	kW - 10 MW			
		Operating temperature	up to 120 °C			
		Round-trip efficiency	>90%			
		Storage period	hh			
		Energy density	56-60kWh/m^2			
		Lifetime (yrs or # of cycles)	300-3000 cycles			
	HT PCM	Range of capacities	10 kWh - GWh			
		Range of power	kW - 100MW			
		Operating temperature	up to 1000 °C			
		Round-trip efficiency	>90%			
		Storage period	hh – dd			
		Energy density	30-85kWh/m^2			
		Lifetime (yrs or # of cycles)	>5000 cycles			
	All latent TES	Cost ($/kWh)		25-90	25-35	<12
		Efficiency roundtrip (%)		>90	>92	>95
	CL TES	Range of capacities	MWh - 100 MWh			
		Range of power	10 kW - 1 MW			
		Operating temperature	500 - 900 °C			
		Round-trip efficiency	45 – 63%			

[1] Latent heat storage: ice thermal storage, sub-zero temperature phase-change materials (SZ PCMs), low-temperature PCMs (LT PCM), high-temperature PCMs (HT PCM)

Type	Technology	Attribute	-	2020	2035	2050
Thermochemical[1]		Storage period	Mm			
		Energy density	800-1200 kWh/m^2			
		Lifetime (yrs or # of cycles)	>30 yrs			
	SH TES	Range of capacities	10 kWh - 100 MWh			
		Range of power	n.a.			
		Operating temperature	30 - 200 °C			
		Round-trip efficiency	50 – 60 %			
		Storage period	Mm			
		Energy density	200-350 kWh/m^2			
		Lifetime (yrs or # of cycles)	20 yrs			
	AS TES	Range of capacities	10 kWh - 100 MWh			
		Range of power	10 kW – 1 MW			
		Operating temperature	5 - 165°C			
		Round-trip efficiency	COP: 0.7 – 1.7			
		Storage period	hh - dd			
		Energy density	180-310 kWh/m^2			
		Lifetime (yrs or # of cycles)	50 yrs			
	All Thermochemical TES	Cost ($/kWh)		n.a.	80-160	<80
		Efficiency roundtrip (%)		n.a.	n.a.	n.a.
Mechanical-thermal coupled systems[2]	CAES	Range of capacities	10 MWh - 1 GWh			
		Range of power	10 – 1000 MW			
		Operating temperature	up to 600 °C			
		Round-trip efficiency	90 % (thermal)			
		Storage period	hh - ww			
		Energy density	n.a.			
		Lifetime (yrs or # of cycles)	40 yrs			
	LAES	Range of capacities	MWh - GWh			
		Range of power	10 – 300 MW			
		Operating temperature	>300 °C (heat), -150°C (cold), -196 °C (liquid air)			
		Round-trip efficiency	90 % (thermal)			
		Storage period	hh – mm			
		Energy density	n.a.			
		Lifetime (yrs or # of cycles)	25 yrs			
	All Mechanical thermal coupled systems	Cost ($/kWh)			400-870	150-260
		Efficiency roundtrip (%)		40-65	45-75	50-80

[1] Thermochemical heat storage: chemical looping (CL TES), salt hydration (SH TES), absorption systems (AS TES)

[2] Mechanical-thermal coupled systems: compressed air energy storage (CAES=, liquid air energy storage (LAES)

6.3 Energy storage models developed in ES TCP Task 32

This section provides a high-level overview of the model frameworks developed in ES TCP Task 32, which can be explored in subsequent work to improve storage modelling in the TIMES framework. The description focuses on the following elements:

- Overview: Short high-level description of the model
- References/Links: listing publications or links useful for readers
- Data inputs: definition of the inputs required to run the model.
- Data Output: definition of the outputs that should be expected by the model.
- Programming language and other characteristics
- Contact information of the colleague involved in the development of the model within the ES TCP Task 32

6.3.1 Compressed Air Energy Storage (CAES)

Overview: It is a toolchain developed to obtain a consistently parametrised storage model. This toolchain is used to derive models for CAES and Pumped Hydrostorage (PHS). It uses detailed simulation models of a particular storage system and, from there, derives a simple reservoir storage model of the same system, which can be potentially used within large energy system models such as TIMES.

The toolchain was applied to an LTA-CAES with 8 compression and 4 expansion stages with an electrical charging power of 53 MW, an electrical discharging power of 32 MW and a storage capacity of 343 MWh, analogues to (Budt, 2016)

The toolchain was used to identify the main influencing factors regarding a reservoir-type model of this CAES, with the main influencing factor for the charging efficiency being the charging power, a COP value of 86.7 %. With COP values of 6.3 % and 8.1 %, respectively, the humidity and the ambient temperature have a negligible influence on the charging efficiency. For the discharging efficiency, only the discharging power is used in the meta-model and, as such, has a COP value at all. The losses during storing, e.g., the storage efficiency, are determined by the initial state of charge at the beginning of the storing process.

References/Links: (Budt, 2016)

Data Inputs: The required input data for the reservoir type model are the maximum charging and discharging power, as well as the maximum storage capacity. The function for the charging and discharging efficiencies and storage losses is obtained with the toolchain and is specific to the storage system analysed.

Data Output: The output of the model is the current operation mode of the storage system in each timestep. Its charging and discharging power in each timestep, as well as the state of charge in each timestep.

Programming language: Python

Contact: E.Schiske, K. Wode, M. Hadam (FhG UMISICHT)

6.3.2 Pump Hydro Energy Storage (PHS)

Overview: It is a similar toolchain as before, developed to derive a model for Pumped Hydrostorage (PHS). It uses detailed simulation models of a particular storage system and, from there, derives a simple reservoir storage model of the same system, which can then potentially be used within large energy system models such as TIMES.

References/Links: (Wode et al., 2023)

Data Inputs: The required input data for the reservoir type model are the maximum charging and discharging power, as well as the maximum storage capacity. The function for the charging and discharging efficiencies and storage losses is obtained with the toolchain and is specific to the storage system analysed.

Data Output: The output of the model is the current operation mode of the storage system in each timestep. Its charging and discharging power in each timestep, as well as the state of charge in each timestep.

Programming language: Python

Contact: E.Schiske, K. Wode, M. Hadam (FhG UMISICHT)

6.3.3 Redox Flow Battery (RFB)

Overview: This model forms the basis of a practical simulation tool for the vanadium redox-flow battery. It comprises a transient, two-dimensional model based on conservation principles (mass, momentum, and charge), incorporating the transport for the charged species and water. This transport model is combined with a kinetic model to simulate the performance of the all-vanadium RFB. The transport of each charged species occurs by diffusion, migration, and convection, and finally contributes to the current and affects the performance. The Vanadium-RFB system involves highly nonlinear terms and coefficients in a complex system of partial differential equations.

They couple the fluid dynamics and electrochemical phenomena. To formulate them, it is necessary to adopt certain simplifying assumptions depending on the number of species and the relative concentrations.

References/Links: (Chakrabarti et al., 2020; Gurieff et al., 2020; Shah et al., 2008)

Data Inputs: cell geometry (negative electrode, membrane, positive electrode), flow rate, current density, electrolyte volume, flow rate, cycle number, charge/discharge time

Data Output: Ion Concentration or potential at constant flow rate mode, cell voltage vs. time curve, charging /discharging profiles

Programming language: COMSOL Multiphysics 5.6 version

Contact: NRC –KR(KIER)

6.3.4 Li-Ion Battery (LIB)

Overview: An online tool (named SoXery) has been developed to evaluate the ageing of a battery, given the usage conditions. The tool is based on a semi-empirical model. It takes the power and temperature profiles of the battery from the user and the chemistry of the cell to calculate the ageing that the cell will undergo over a certain period. The output from the tool includes the calendar and cycle ageing in the cell, the increase in the internal resistance of the cell as well as an unfulfillment map, which shows whether the cell was able to adhere to the usage profile or not. The tool is intended to be used as a first approximation by users who want to know the most appropriate cell chemistry given a usage profile or for sizing their battery for a specific purpose. Many types of battery models exist. They can be broadly divided into (i) Electrochemical models, (ii) Electrical models, (iii) Analytical models and (iv) Stochastic models.

The model developed here consists of two parts: i) dynamics model and ii) degradation model. The dynamics model governs the voltage, internal resistance and soc change during charging and discharging. It is based on a simple equivalent circuit model consisting of a voltage source and a variable resistor.

The degradation model describes the calendar and cycle of ageing that the cell will undergo during its lifetime. It is based on a semi-empirical stress factor model. The SoC and temperature are assigned as stress parameters for calendar aging, while C-rate, temperature, average SoC and DoD are assigned as stress parameters for cycle aging. The aspects of calendar and cycle aging apply to both SoH decrease as well as SoR increase, although in different proportions given by experimental data. The values of the stress factors determine the cell's degradation rate, and thus, the total degradation in each time period can be computed.

Simulations are carried out at the cell rather than the battery pack level.

References/Links: (Bhoir et al., 2021; Xu et al., 2018)

Data Inputs: timeseries with battery power to be injected, battery load at each timestep, temperature profile, size of the battery pack, cell chemistry and the minimum and maximum SoC allowed during the simulation, resistance-SoC-Temperature map.

Data Output: degradation (total or cycling and calendric) causing a decrease of SOH and/or increase of SOR (rate of resistance) over the simulation period, estimated SOC profiles, power output/input (Watts) during discharge/charge, unfulfillment of the requested profile due to SoC limits.

Programming language: Python for the code available online at GitHub (https://gitlab.ti.bfh.ch/oss/esrec/open-sesame.git), SoXery for the GUI (www.tinyurl.com/soxery). The user must provide the profile parameters and battery parameters (see above). A user guide explaining these parameters in depth is also provided on the SoxeRy website.

Contact: P. Caliandro C. Brivio (ESReC, BFH+CSEM)

6.3.5 Li-Ion Battery (uCalgary)

Overview: It is a computationally attractive linearised physics-based model that is introduced to improve the accuracy and feasibility of the lithium-ion battery energy storage system operation strategy. It captures many details of the operational characteristics of LIBESS, which are usually formulated using coupled partial differential equations and various nonlinear algebraic expressions. Instead, mixed-integer linear programming is formulated in this Li-Ion Battery model, which can be solved using commercial off-the-shelf solvers. Piece-wise linearisation and Taylor series expansion techniques approximate the non-linear equations.

The model's focus is LIBESS's short-term operation. The optimisation problem is an energy arbitrage strategic operation: LIBESS is a price-taker, and no uncertainty is considered. The objective of the LIBESS owner is to maximise profit by trading energy over the 24-hour interval. The cost of degradation is included through the energy throughput quantification technique. The constraints of the optimisation problem correspond to the proposed LIBESS formulation.

References/Links: (Ning & Popov, 2004; Subramanian et al., 2001; Vykhodtsev et al., 2024)

Data Inputs: To build a proposed linearised physics-based lithium-ion battery model, a set of parameters for underlying electrode chemistry is needed. To build an optimisation framework, a set of market data is required. The latter include hourly electricity mixes and prices**.**

Data Output: The output is the dispatch of LIBESS for the energy arbitrage operation.

Programming language: The optimisation framework was formulated using Julia programming language and it was solved employing Gurobi Optimizer 9.1.2 solver.

Contact: A. Vykhodtsev (uCalgary + NRC)

6.3.6 Li-Ion Battery (NRC) – equivalent circuit model

Overview: The NRC Li-Ion battery model can be separated into two distinct portions: the electrical model and the thermal model. The electrical model consists of an equivalent-circuit model, which is not meant to describe the construction of the cell; rather, it acts as a description of the cell's high-level behaviour. The various components used to build this model (resistors, capacitors, etc…) are not actually present in the cell but do act as analogues for some of the internal processes. The thermal model for the battery is a physic-based model that assumes the primary heat generator in the cell can be attributed to Joule heating. The model uses Joule's law to calculate the power generated due to resistance, which is proportional to heat flow from the resistor if it is assumed that all electrical losses in the resistor are converted into heat. This model then builds the physical layers for the cells and the pack and assumes perfect heat conduction between each layer of the cell. The model is used for an NMC cells but should be valid for most chemistries; it would simply require a retuning of the parameters.

Electrical model: The cell discharge model was an equivalent-circuit model (ECM). More specifically, it was an enhanced self-correcting model structure, which included the following effects: Open-circuit voltage (OCV), State-of-charge (SOC) dependence, Temperature dependence, Equivalent circuit resistance, Diffusion voltages, Hysteresis voltages. To develop an ECM, it is necessary to first describe open-circuit voltage (OCV) theory. The model is first built to represent the cell as an ideal voltage source. This type of model alone is not accurate enough for most applications, as in reality, cell voltage is dependent on the load current, recent usage, ageing, and many other factors. However, an accurate OCV is still the base upon which the rest of the model is built.

Thermal Model: The thermal component of the NRC model is specific to the NRC's hybrid-electric aircraft battery as it is entirely physic-based. However, the process by which it was designed can be relatively generalised and will be summarised here. The NRC model assumes that the primary source of cell heating is Joule heating and that the source of the heat generation is located at the geometric centre of the cell. The model is assumed to be prismatic in construction and requires the following specifications: Nominal Voltage, Nominal Capacity, Max Voltage, Length, Width, Depth, Weight, Specific Heat Capacity, and Thermal Conductivity. These are defined for each thermal interface between the core of the cell and the external surfaces.

References/Links: (Gregory L. Plett, 2015)(Lidbeck & Syed, 2017)

Data Inputs: Parameters describing the cell chemistry (separately for each cell, such as resistance, capacity, etc.), the material properties required for the thermal model (density, thickness, specific heat capacity, thermal conductivity), as well as the geometric properties of the cells to be modelled (cell dimensions, material properties).

Data Output: The electrical component of the NRC model can provide discharge and charge performance (voltage, SOC) reasonably well in many scenarios with proper tuning. When coupled with the thermal model, it can also provide insight into the performance of a given cooling solution. The models cannot provide information on the physical aspects of Li-Ion cells, such as degradation due to use in cold or hot temperatures or due to ageing effects. The model is suitable for short-term simulation goals in a dynamic system and has not been validated for long-term simulations.

Programming language: The model was developed in the Modelica language using the Dymola interface. The parameter tuning was done using Python 3.9.9 and the scipy.optimize.minimize() function. The model was tuned and validated for a hybrid electric aircraft and needs to be validated for use in grid applications.

Contact: A. Crain, D. Jang (NRC)

6.3.7 Li-Ion Battery (NRC) – Surrogate model

Overview: The NRC machine learning model is a battery cell surrogate model for voltage estimation using deep learning methods. In this case, 'surrogate' refers to the fact that the model is intended to act as a complete black box model and does not include any true physics. The model was developed to estimate cell voltage at a given current, state of charge (SOC), and temperature operating condition. The deep learning modelling framework provided the ability to capture the intricacies of the battery cell behaviour without the need for computationally expensive analytical equations and without the requirement for an in-depth understanding of the electrochemical processes occurring within the cell. Two models were developed: the first being a standard gated recurrent unit (GRU) network implementation, and the second being a GRU implementation with transfer learning. The first model was trained exclusively using experimental data collected in the ground testing campaign of the Hybrid-Electric Aircraft Testbed (HEAT) II project. This campaign consisted of a variety of performance tests in which the battery was discharged across a large portion of its operational range. The model was observed to perform well with respect to its training and validation losses but was visibly lacking in accuracy at low state of charge conditions due to lack of experimental data. The second model was developed using transfer learning to reduce the first model's deficiencies within the low state of charge regions. The model was pre-trained on a large, simulated data set generated from a Modelica equivalent circuit model, and transfer learning was applied to transfer the weights to a new model, which was further trained on the smaller experimental dataset. Marginal improvement was realized by the transfer learning model. However, the estimations at a low state of charge continued to be slightly inaccurate.

The data was split into training, validation, and test sets, each consisting of 70%, 20%, and 10% of the overall dataset, respectively. Deep learning datasets typically use a much higher proportion of the data for training (often above 95%). However, since only 34 discharge curves were available, it was desirable to have sufficient data in the validation and test sets to prevent the model from overfitting.

The most obvious deficiency in the model was the lack of training data available. Specifically, the shortage of data at a low state of charge was found to limit the model's performance. For improved performance, it is recommended that additional data be collected across the operational range of the cell, with emphasis on low state of charge performance.

References/Links: (Crain et al., 2021; Doetsch, 2020)

Data Inputs: To run this model, the current load (in amps), the current state-of-charge (in percent), and the current temperature (in degrees Celsius) are re-quired. These requirements also apply to the training set requirements should the model need to be retrained.

Data Output: The model estimates the cell voltage at the same time step as the inputs, but accounting for the voltage decrease/increase due to cell temperature and load.

Programming language: This model was developed using Python 3.9.9 and the TensorFlow 2.0 API.

Contact: A. Crain, D. Jang (NRC)

6.3.8 Li-Ion Battery (NRC) – NARX State-of-Charge Predictor

Overview: This model uses the active power command and the state-of-charge for the current time-step and implements a nonlinear auto-regressive network with exogenous inputs to predict the state-of-charge at the subsequent time-step. The neural network training algorithm is written in the Julia programming language, independent of any existing machine learning platforms; the resulting model is compared to one developed using Python/TensorFlow. The simulation performance was validated with data collected from the energy storage system that was dispatched to follow a standard frequency regulation duty cycle not used as part of the training data. The mean-absolute-error between the predicted state of charge and the validation data is shown to be less than 1%, despite the limited data and lack of physical information about the system.

More specifically, data from a Tesla PowerPack 2 - used to provide auxiliary power to the Wind Energy Institute of Canada's (WEICan) 10 MW wind farm – was used for the development of this model. WEICan does not possess any models for their ESS – which could be used for predicting the impact of varying loads on their ESS – and are also limited in the data they can collect for the development of such a model. The original publication (accepted but unpublished at this time) focuses on the code development as well as the resulting model.

The input to the model is the active power at a given time-step. The model then predicts the state-of-charge at the next time-step. The initial SOC is set to be the first point in each training set, and active power is taken from the data directly for each point. The model knows nothing about the inner workings of the ESS or inverter, and thus is expected to include all losses in the system. Selection of the number of layers and nodes, as well as the activation functions, was done incrementally by increasing both gradually and assessing the impact on the training and validation cost curves.

Both models show larger errors around high active power demand segments, indicating that they did not adequately generalise for extrapolation into power ranges outside the training set. To improve the generalisation, this model could be trained on more data, or alternative structures could be tried, such as an adversarial network.

References/Links: (Crain et al., 2023)

Data Inputs: For model training, the following inputs are required**:** Active Power (kW) Data at Time-Step i, State-of-Charge (%) Data at Time-Step i+1. For model inference, the following inputs are required: active Power (kW) Time-Step i.

Data Output: When training the model, the output are the weights and biases for the neural network. When running the model in inference mode (prediction), the output is the state of charge at the next time step (i+1).

Programming language: The Julia model was developed using in-house software developed on Julia 1.8.0. The TensorFlow model (for validation) was developed using Python 3.9.9 and the TensorFlow 2.0 API

Contact: A. Crain, D. Jang (NRC)

6.3.9 Na-Ion Battery

Overview: The Na-Ion Battery Model is an integrated modelling framework for assessing the performance, costs, and environmental impacts of Lithium-Ion-Batteries (LIB) and Na-Ion-Batteries (NIB) cells. It consists of (1) a physics-based pseudo-two-dimensional (P2D) battery cell model to assess the performance of battery cells subjected to varying discharge rates, (2) a bottom-up battery cell cost model, and (3) a model to quantify the environmental impacts of battery cells based on life cycle assessment.

The P2D battery cell model, based on porous electrode theory[a], assesses the practical, specific energies of intercalation-based LIB and NIB cells under varying discharge rates. The P2D model is represented by a system of coupled nonlinear partial differential equations for the conservation of mass and charge in the three main sections of the battery cell: cathode, separator, and anode. The P2D model is coupled to an optimisation solver to numerically optimise the cell design parameters for maximum practical, specific energy at different discharge rates.

The practical, specific energies and optimised LIB and NIB cell designs from the P2D model constitute the basis for the computation of material requirements used to assess costs and manufacturing-related life cycle GHG emissions of a typical size of 1kWh battery cell capacity without consideration of the battery use phase and end of lifetime aspects. The assessment of the manufacturing costs is based on a bottom-up cost model. The total manufacturing costs are the sum of material purchase, process, and overhead costs. Learning curves are also considered when computing the battery process and overhead costs. While material purchase costs can be directly computed from the output of the P2D model, the process costs are estimated based on the assumption that the production line occupation times are inversely proportional to the areal-specific energy of the electrode sandwiches of the battery cells composed of. The process costs also include a constant term as well.

In calculating the environmental impacts via life cycle assessment (LCA), the greenhouse gas emissions (GHG) are computed according to IPCC 2013 (100-year time frame) using the Python-based Brightway LCA framework. The Ecoinvent database version 3.3 provided the background GHG emissions of all modelled battery materials, and energy carriers needed to manufacture the cells. All calculations were performed for battery cells in a standard industrial pouch format, where multiple electrode sandwiches consisting of an anode current collector, anode, separator, cathode, and cathode current collector are stacked on top of each other. Due to the unavailability of industrial data, it is assumed that the thickness of the NIB anode aluminium current collector is equal to the thickness of the LIB anode copper one. However, it should be noted that this assumption is possibly favouring NIBs, as it is currently unclear whether the mechanical stability of aluminium allows for the processing of aluminium sheets with a thickness of only 8 μm. A scrap rate of 9% is assumed for all components of the battery cell sandwich.

References/Links:

[1] S. F. Schneider, C. Bauer, P. Novák, and E. J. Berg, Sustainable Energy & Fuels, 2019, 3, 3061-3070

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Data Inputs: The main physicochemical input parameters for the integrated modelling framework of LIB and NIB battery cells are Li+ and Na+ concentrations in active materials and electrolytes, solid phase diffusion coefficient of Li+ and Na+, heterogeneous reactions rates at anode and cathode, particle radius of anode and cathode, the gravimetric density of anode and cathode current collector, the gravimetric density of anode and cathode active material, density of electrolyte, electronic conductivity of anode and cathode composite materials, and Bruggeman coefficient in the cathode, separator and anode.

Data sets for assessing life cycle GHG emission were adapted from a general LIB inventory source using ecoinvent version 3.3 as a background database. The database considers several materials and processing steps while manufacturing the LIB and NIB cells, together with related GHG emissions. Reference prices of materials are obtained from the literature.

Data Output: The framework produces as outputs projected practical, specific energies for LIB and NIB cells for different discharging rates. Serving as a first validation, the model's output is benchmarked against the practical, specific energies of LIB cells used in electric vehicles. In addition, the model projects battery cell costs by component and GHG emissions related to their manufacturing.

Programming language: The P2D model is programmed in MATLAB. The bottom-up cost optimisation model is based on EXCEL. The Lifecycle model is based on Python.

Contact: E. Panos (PSI)

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