The CompBat project - **WHAT WE DO**

An overview of research activity

Electrical energy storage is one of the key challenges to address to realize the green transition to a low-carbon economy. An extensive storage capacity will be required to balance the fluctuating nature of variable renewable energy sources such as wind and solar.

Redox Flow Batteries (RFBs) are a promising option for large scale stationary energy storage. RFBs utilize redox-active materials dissolved in liquid electrolytes stored in tanks, and the amount of the stored energy depends on the volume of the tanks. Pumps ensure the circulation of the electrolytes through electrochemical cells where the electrochemical reactions take place.

RFBs have a great potential for stationary applications, due to a set of features such as the possibility to decouple energy (tank size and amount of electrolyte) and power (cell surface and pumped mass flow) thanks to their modular nature which makes them extremely flexible and scalable in design. In addition, it is possible to fully recover performance losses with time and number of cycles, up to nominal conditions with moderate maintenance. Finally, the lifecycle that they can reach is long, above 10000 cycles which may easily mean ten to twenty years thanks to the already reached stability of the redox-active materials.

State-of-the-art of RFBs work with non-flammable aqueous electrolytes utilizing highly acidic solutions based on vanadium sulfates. On the one hand, vanadium is recyclable and not scarcely present on earth as lithium, therefore if properly recycled it would lead to a lower environmental footprint. On the other hand, it would be better to develop the RFBs working with non-corrosive solutions and based on ubiquitous materials such as organic molecules or non-toxic metals. This could boost a large scale deployment because it would dramatically reduce its price and environmental impact, plus reduce the dependence of European Union from importing vanadium.

Affordable RFBs based on renewable or abundant raw materials are therefore urgently needed. The potential energy storage materials are chemicals that need to fulfil several criteria, including a reasonable high energy density, stability, and production at an affordable cost, but no such chemicals have been discovered yet. To contribute towards solving this problem, CompBat will focus on developing tools for the discovery of new prospective candidates for next-generation flow batteries, based on machine learning assisted high-throughput screening. Density functional theory calculations will be used to obtain data on solubilities and redox potentials of different molecules, and machine learning methods are used to develop high-throughput screening tools based on the obtained data.

The results of the high-throughput screening are validated with experimental results. Target molecules will be bio-inspired organic compounds, as well as derivatives of the redox-active chemical species already manufactured in bulk quantities. We propose to use safe and inexpensive natural products, such as vitamins and amino acids as building blocks for aqueous flow battery materials operating close to neutral pH. The advantages of natural product derived materials include: 1) scalable production in tanks by fermentation with reasonable cost, 2) inherent safety and expected biodegradability due to their biological origin and natural roles even in the human body, 3) solubility in water, and 4) high degree of functionalization, minimizing the need for synthetic steps to modify them.

As next step, numerical modelling of flow battery systems will be performed with finite element method enabling to investigate cell details and provide the required information to develop more general zero-dimensional models based on mass-transfer coefficients. The latter would enable faster and reliable simulations of the cells performance that could be verified with the first ones. Both models will also be validated experimentally and used for generating a data-set to allow prediction of the flow battery cell performance based on properties of the prospective candidates obtained from high throughput screening.

Finally, cells will be piled in stacks reaching higher power values and modelled to understand the effect of parasitic shunt currents, as well as including the effect of other components as pumps and tanks. Furthermore, the battery performance will be enhanced by the use of solid boosters, to be manufactured from inexpensive and abundant raw materials. Solid boosters consist of particles introduced into the flow battery solution tanks as beads composed only of the active material, conductive additive and binder. Due to the reaction between the solid particles and the active components present in the electrolyte, the dissolved redox species, the storage capacity will be enhanced only at the extra cost of the raw materials. In fact, the amount of electrolyte will be the same, and the limiting factor to the capacity will no longer be the solubility of the dissolved species determining a higher energy density than that of the conventional RFBs.

This data is used then to predict the flow battery overall system performance. In this way, including economic assumptions, it will be possible to develop tools capable of assessing the battery costs and stored energy cost, such as the Levelized Cost Of Storage (LCOS). So techno-economic studies could be performed, comparing different solutions in terms of storage technology and energy system integration, as well as identifying suitable targets for the RFBs development.

PARTNER 1- **Research Centre for Natural Sciences TTK, Hungary**

STEP 1 - TTK Research Centre of Natural Sciences

ABSTRACT

1. **Bioinspired molecules** derived from vitamins and amino acids are promising class of compounds for novel redox flow batteries.

2. **Molecular design** via systematic variation of functional groups is the initial step in establishing high-throughput screening (HTS) methods.

3. Accurate **quantum chemical calculations** provide a benchmark database for redox potentials and water solubilities.

4. **Machine learning** approaches serve to accelerate the discovery of new redox active materials.

5. The developed **HTS tool** enables the identification of promising candidates for synthetic and electrochemical studies.

PARTNER 2- **Aalto University, Finland**

STEP 2 - AALTO

ABSTRACT

1. Quantum mechanics based simulations for studying the electron transfer from electrode to molecules. We can obtain the reaction energies and barriers. (related to parabola figure in left)

2. The simulations are based on ab initio molecular dynamics and Constrained Density Functional Theory (cDFT). (figure related to cDFT)

3. The electron transfer is modelled using the Marcus theory. The cDFT simulations will provide parameters for the Marcus equation. (figure related Marcus theory and cDFT)

4. Various charge states and transition between them has been modelled. (figure redox reactions)

5. Slow electron transfer can make the RFB inefficient. At the moment very little is known of the electrode to molecule charge transfer. Such simulations have not been done before and experimentally the charge transfer is difficult to measure. (general motivation)

PARTNER 3- **University of Jyväskyla, Finland**

STEP 3 - JYVÄSKYLÄ

ABSTRACT

1. The choice of the molecules to be synthesized is guided by the results of computations from TTK and Aalto.

2. The starting materials are allowed to react, and the product is isolated.

3. Purification of the products is carried out by different purification techniques.

4. The pure products are then characterized by measuring their NMR spectra.

5. Additional characterization with mass spectrometry and elemental analysis gives additional certainty to the molecular structure.

PARTNER 4- **University of Turku, Finland**

STEP 4 - TURKU

ABSTRACT

1. Electrochemical testing of new molecules to measure their electrochemical properties to evaluate their suitability for batteries. This data is needed to validate computational results from TTK.

2. Initial battery testing of the new molecules to evaluate their stability under operating conditions. This data is utilized to validate models developed by UPPSALA and SKOLTECH.

3. Further battery testing to evaluate the performance of the new molecules in a battery. This data is utilized to validate models developed by SKOLTECH and UNIPI.

PARTNER 5- **Uppsala University, Sweden**

STEP 5 - UPPSALA

ABSTRACT

1. The main objective of UU is the development of a **FEM model** for a redox-flow battery, describing the electrochemistry and predicting the voltage and current generation with parameterization coming from DFT and experimental inputs.

2. **Parametric sweep** is performed for a refinement of the flow cell model. Generated data is compared with experimental results and identifying the most significant parameters, potential hotspots and the domains were improvements are necessary.

3. Development of an electrochemical model for a packed bed reactor filled with a **solid booster**. In this step, a model for solid redox species will be included based on conventional battery types.

4. Coupling the solid booster model with the flow battery model will be implemented, evaluating of different parameters on the battery performance. All the generated data will be used for the development of the 0D model in WP3.

PARTNER 6- **Skolkovo Institute of Science and Technology, Russian Federation**

STEP 6 - SKOLTECH

ABSTRACT

1. The data from 2D simulations are further simplified and used for 0D dynamic modeling of a single-cell RFB system.

2. **The dynamic simulations** of a single cell RFB systems under different operating conditions (e.g. loading currents, flow rates) are performed also considering systems with solid boosters. The simulations are validated with the experimental data.

3. **The analysis of total losses** is performed and simplified efficiency indicators are derived for techno-economic studies to determine the most prospective candidates among the discovered redox couples.

PARTNER 7- **Università di Pisa, Italy**

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 875565. The content on this document represents the views of the authors, and the European Commission has no liability in respect of the content.