

DELIVERABLE REPORT

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1 Introduction

This document describes the first version of the optimized techno-economic model that was developed. A detailed cost analysis of different flow battery types served as the basis for a structured evaluation of the cost distribution of the battery system and as a basis for the techno-economic modeling of these batteries. These were also built on a laboratory scale for the purpose of validation measurements and collection of the performance data to be represented in the model, and their structure was recorded in all components (technical and non-technical).

In addition to inorganic vanadium flow batteries, organic methyl viologen (MV)/4-hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPOL) flow batteries were built and modeled.

Techno-economic models are a means that helps to capture and analyze systems simultaneously under technical and economic aspects. The simultaneous consideration of both technical and economic parameters can be understood as an extension of the system boundaries [1].

For this purpose, a techno-economic model [2] for flow batteries developed at the ICT was further developed to better represent the technical properties of different active materials and electrolytes with regard to the battery model and the factors influencing costs. From the specification of the required power and energy of a flow battery system, the model can calculate the quantity of components required and the resulting cost based on the internal resistance of the battery. Both material and manufacturing costs are considered. This representation of CAPEX was created in the first step based on the flow batteries built at ICT itself and comprehensively recorded in terms of costs and performance on a laboratory scale.



The model was developed in several steps:

- 1) Acquisition of all components (technical and non-technical) of the flow battery on a laboratory scale;
- Standardization of all components, with the exception of the electrolyte used, to ensure the best possible comparability of the various inorganic and organic flow batteries;
- 3) Recording of the performance parameters of the standardized flow batteries built in this way along likewise standardized series of tests;
- 4) Mapping of both the technical (electrochemical) functions and the cost functions;
- 5) Integration of costs collected during construction and performance data measured in the laboratory into the techno-economic model.

Using this model, techno-economic sensitivity analyses were then carried out on a component-by-component basis to be able to estimate, among other things, the optimization potential of these components for the entire flow battery.

2 <u>Hierarchical model of the standardized flow battery</u>

2.1 General assumptions

The model is based on the following assumptions:

- First of all, flow batteries are to be built on a laboratory scale and a standard is to be defined that can be used for both inorganic vanadium flow batteries and organic flow batteries;
- All components required in the construction and operation of the flow battery are to be recorded. This includes both technical and non-technical components;
- If possible, the recorded components are to be sorted or grouped along higherlevel criteria.

This purely mapping model is the basis on which the individual components are then mapped in the techno-economic model in terms of their influences, both quantitative and qualitative, on the costs and performance data of the flow battery.

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2.2 FlowBatterie

The vanadium flow battery was chosen as a starting point because it has been well researched for decades [3,4,5].

In this project, a flow battery is understood as consisting of 2 corresponding half-cells, in each of which an electrochemical reaction of a RedOx pair takes place. During operation, the posolyte and negolyte, which are stored separately in tanks, are pumped into the cell, each of which they flow through in one of the two half-cells separated by a membrane. The electrochemical reaction required during charging and discharging then takes place in the cell. The anode and cathode, where the oxidation and reduction take place, respectively, change depending on whether the battery is in charging or discharging mode.

The reversible cell voltage results from the potential difference of the two half cells.

In the vanadium flow battery, the tetravalent VO^{2+} species are oxidised to pentavalent vanadium (VO_{2^+}) during the charging process in the posolyte at the positive electrode. In the negative half cell, V^{3+} ions are reduced to VO^{2+} ions, as can be seen in **Figure 1**.

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Figure 1. Schematic representation of the charging and discharging process of a flow battery using the example of a vanadium flow battery (VFB).

2.3 <u>Hierarchical component model of a flow battery on a laboratory scale</u>

During the construction and standardization of various flow batteries on a laboratory scale, a hierarchical component model was developed.

The technical components used in the standardized flow battery and the working time required for the construction were used as a basis. The cell structure is shown in **Figure** 2.

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Figure 2. Schematic diagram of the structure of the standardized laboratory cell with (1) end plate, (2) insulation plate, (3a and b) fittings and tube sealing caps, (4 and 10) gasket, (5) current conductor, (6) gas diffusion layer, (7) bipolar plate, (8) flow frame, (9) electrode, and (11) membrane.

The electrolytes are pumped through this cell in separate circuits from their respective tanks. The overall structure of such a flow battery on a laboratory scale can be seen in **Figure 3**.

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In addition to the technical components required for the construction of such a flow battery, the non-technical components, such as the time required for construction, were also recorded to be able to represent such costs in the model in the following.

All these components were also grouped and assigned to different hierarchies whenever possible during the creation of the model. The guiding question in this horizontal as well as vertical classification was: "Which desired output of the flow battery is this component significantly conducive to?"

On the one hand, the flow battery has the ability to store energy. This takes place primarily in the electrolytes, so that the tanks in which these electrolytes are stored and the electrolytes themselves were assigned to the Energy area. In addition, it was mapped hierarchically that an electrolyte regularly consists of the active species, the solvent and, if required, an additive. These electrolytes usually are to be manufactured in the laboratory, so that these costs are also shown as a non-technical component.

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In addition, flow batteries must also be able to absorb or deliver electrical power. This is done in the cell, or if several cells are installed, in the stacks. All the components required for the construction of the laboratory cell (see **Figure 2**) are therefore assigned to the Power section. The wiring required to complete the circuit and the assembly of the cell or, if applicable, the stacks are also assigned to this area.

Components that cannot be assigned to either Energy or Power and are necessary for controlling or operating the battery can be found in the Control & Connect area. The final assembly of the entire FlowBattery, i.e. the connection of the other two areas, is also shown there.

The resulting hierarchical component model is shown in Fehler! Verweisquelle konnte nicht gefunden werden..

The technical components used in the laboratory-scale standardized flow battery are listed in

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The technical components used in the standardized flow battery on a laboratory scale

| are | | listed | in | | | | | | |
|-----------------------|---|------------------------------------|--|--|------------------------|--|--|--|--|
| | | | Component | | | | | | |
| 1 st Order | 2 nd Order | 3 rd Order | Vanadium FB | MV/TEMPOL FB | | | | | |
| Energy | | | | · | | | | | |
| | Tank _{Negolyte} | | screw top bottles (DURAN GL multiple distributor (Carl Roth v | 45) vith four threaded necks) | | | | | |
| | Negolyte | | DegraBat-II Vanadiumelectroly | rte | | | | | |
| | | Active Species _{Negolyte} | V ^{3.5+} | Methylviologen 1,1'-Dimethyl-4,4'-bipyridinium-dichlorid Hydrat | AQS anthraquinone | | | | |
| | | Solvent _{Negolyte} | Sulfuric acid | SodiumChlorid | Sulfuric Acid | | | | |
| | | Additive _{Negolte} | Phosphoric acid | | | | | | |
| | | Fabrication _{Negolyte} | | Time _{required} : 20 min Rate _{hourly} : 30 €*h ⁻¹ | | | | | |
| | Tank _{Posolyte} | | screw top bottles (DURAN GL multiple distributor (Carl Roth v | 45) vith four threaded necks) | | | | | |
| Posolyte | | | DegraBat-II Vanadiumelectroly | rte | | | | | |
| | | Active Species _{Posolyte} | V ^{3.5+} | 4-OH-TEMPO 4-Hydroxy-2,2,6,6-tetramethylpiperidinyloxyl | BQDS 1,2-Dihydroxyt | | | | |
| | | Solvent _{Posolyte} | Sulfuric acid | SodiumChlorid | Sulfuric Acid | | | | |
| | | Additive _{Posolyte} | Phosphoric acid | | | | | | |
| | Tank _{Posolyte} Posolyte Posolyte Solation plate Endplate Connection Final Stack Assembling Cell | Fabrication _{Posolyte} | | Time _{required} : 20 min Rate _{hourly} : 30 €*h ⁻¹ | | | | | |
| Power (Stack) | | | | • • | | | | | |
| | Current collector | | copper foil (Schlenk Cu-ETP F | 3200) | | | | | |
| | Isolation plate | | teflon plate | , | | | | | |
| | Endplate | | aluminium plate | | | | | | |
| | Connection | | test and connecting leads, allig | ator clips, coupling adapter (Bürklin) | | | | | |
| | Final Stack Assembling | | Time _{required} : 40 min Rate _{hourb} : 30 €*h ⁻¹ | | | | | | |
| | Cell | | | | | | | | |
| | | Membrane | Fumasep FAP-450 | | | | | | |
| | | Electrode | SIGRACELL battery felt (GFD | 4.6 EA from SGL Carbon) | | | | | |
| | | Gasket inside | Ice cube sealing (QuinTech 35 | FC-PO 100 0,5) | | | | | |
| | | Cellframe, Channel, Manifold | teflon frames and plates (man estimated Time _{required} : 20 hours | ufactured at ICT) s | | | | | |
| | | Screws | | | | | | | |
| | | Carbon paper | Gas Diffusion Layer without M | PL + PTFE (QuinTech GDS090S) | | | | | |
| | | Fittings | PFA fittings / pipe connectors | (EM- Technik 2N100MN0318PF, 2N100P0503PF, | PFA-220-C) | | | | |
| Control & Connect | | | | | | | | | |
| | Pump | | diaphragm dosing pump (KNF controller 2-phase stepper (KN bench top power supply (Maps | PL6737-FEM 1.09) IF FE Z4) con SSP-7080) | | | | | |
| | Pining | | DEA tubos (EM Toobrik SI 10 | 0\$05EE10 or \$1,100\$01EE10) | | | | | |
| | | | Time _{required} : 20 min | 0303FF10013L100301FF10) | | | | | |
| | Final Battery Assembling | | Rate _{hourly} : 30 €*h-1 | | | | | | |
| | · · | | • | | | | | | |

Table 1.

The successful standardization is shown by the fact that most components are identical for all flow batteries listed. The only differences are in the area of electrolytes.

For the vanadium flow batteries, the electrolyte DegraBat-II from GfE Metalle und Materialien, which has already been produced, was used both as a posolyte and as a negolyte. It consists of a mixture of the compounds $V_2(SO_4)_3$ and $VOSO_4$ with a vanadium concentration of 1.67 mol L⁻¹, 3.8 M sulfuric acid as a solvent and 0.05 M phosphoric acid as an additive. Accordingly, no manufacturing costs were incurred.

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The electrolytes of the MV/TEMPOL and AQS/BQDS flow batteries did not contain any additive.

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Figure 4. Hierarchical component model of a laboratory-scale flow battery, incl. technical and non-technical components.

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| | Component | | | | | | | | |
|-----------------------|--------------------------|---|--|--|--|--|--|--|--|
| 1 st Order | 2 nd Order | 3 rd Order | Vanadium FB | MV/TEMPOL FB | AQS/BQDS FB | | | | |
| Energy | | • | | | • | | | | |
| | Tank _{Negolyte} | | screw top bottles (DURAN GL 45 multiple distributor (Carl Roth with | i) n four threaded necks) | | | | | |
| | Negolyte | | DegraBat-II Vanadiumelectrolyte | | | | | | |
| | | Active Species _{Negolyte} | V ^{3.5+} | Methylviologen 1,1'-Dimethyl-4,4'-bipyridinium-dichlorid Hydrat | AQS anthraquinone-2-sulfonic acid | | | | |
| | | Solvent _{Negolyte} | Sulfuric acid | SodiumChlorid | Sulfuric Acid | | | | |
| | | Additive _{Negolte} | Phosphoric acid | | | | | | |
| | | Fabrication _{Negolyte} | | Time _{required} : 20 min Rate _{hourly} : 30 €*h ⁻¹ | | | | | |
| | Tank _{Posolyte} | | screw top bottles (DURAN GL 45 multiple distributor (Carl Roth with | 5) n four threaded necks) | | | | | |
| | Posolyte | 1 | DegraBat-II Vanadiumelectrolyte | | | | | | |
| | | Active Species _{Posolyte} | V ^{3.5+} | 4-OH-TEMPO 4-Hydroxy-2,2,6,6-tetramethylpiperidinyloxyl | BQDS 1,2-Dihydroxybenzene-3,5-disulfonic acid disodium salt monohydrate | | | | |
| | | Solvent _{Posolyte} | Sulfuric acid | SodiumChlorid | Sulfuric Acid | | | | |
| | | Additive | Phosphoric acid | | | | | | |
| | | Fabrication _{Posolyte} | | Time _{required} : 20 min Rate _{hourly} : 30 €*h ⁻¹ | | | | | |
| Power (Stack) | | · | | | | | | | |
| | Current collector | | copper foil (Schlenk Cu-ETP R200) | | | | | | |
| | Isolation plate | | terion plate | | | | | | |
| | Endplate | | aluminium plate | | | | | | |
| | Connection | | test and connecting leads, alligate | or clips, coupling adapter (Bürklin) | | | | | |
| | Final Stack Assembling | | Time _{required} : 40 min Rate _{hourty} : 30 €*h ⁻¹ | | | | | | |
| | Cell | | | | | | | | |
| | | Membrane | Fumasep FAP-450 | | | | | | |
| | | Electrode | SIGRACELL battery felt (GFD 4. | 6 EA from SGL Carbon) | | | | | |
| | | Gasket inside | Ice cube sealing (QuinTech 35 FC | 5-PO 100 0,5) | | | | | |
| | | Cellframe, Channel, Manifold | teflon frames and plates (manufa estimated Timerequired: 20 hours | ctured at ICT) | | | | | |
| | | Screws | loquiou | | | | | | |
| | | Carbon paper | Gas Diffusion Laver without MPL | | | | | | |
| | | Fittings | PFA fittings / pipe connectors (EM- Technik 2N100MN0318PF, 2N100P0503PF, PFA-220-C) | | | | | | |
| Control & Connect | | | · · · | | | | | | |
| | Pump | | diaphragm dosing pump (KNF PL controller 2-phase stepper (KNF I bench top power supply (Manson | .6737-FEM 1.09) FE Z4) SSP-7080) | | | | | |
| | Piping | | PFA tubes (EM-Technik SL100S | 05PF10 or SL100S01PF10) | | | | | |
| | Final Battery Assembling | Pabrication _{keegevin} Imme _{requine} : 20 min Rate _{room} ; 30 € th ¹ screw top bottles (DURAN GL 45) multiple distributor (Carl Roh with four threaded necks) BODS DegraBal-IV anadumelectivity I BODS Active Species _{Poscopte} V ^{3.5} 4-0H-TEMPO Solvent _{poscopte} Suffaric acid SolumChorid Suffaric acid disodium salt monbyd Additive <u>poscopte</u> Phosphoric acid Suffaric acid Suffaric acid Fabrication _{Poscopte} Phosphoric acid Time _{requine} : 20 min Rate _{room} ; 30 € th ¹ | | | | | | | |

Table 1. List of technical and non-technical components of a flow battery on a laboratory scale.

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3 <u>Techno-economic model of the standardized flow</u> <u>battery</u>

3.1 <u>Measurements to determine the performance parameters of the flow batteries</u> to be modeled

In the laboratory, several flow batteries of the two types vanadium/vanadium and MV/TEMPOL were built and measured, again using standardized test series. In this way, among other things, the performance data of the respective flow battery type required for optimization of the techno-economic model were determined statistically as a mean value including standard deviation.

A selection of the relevant test parameters is listed for the different flow batteries (see **Table 2**, **Table 3**, and **Table 4**).

| Molarity Active Ma | terial Vanadiu | m ′ | 1.67 M | | Vanadium | Vana | dium |
|--|--------------------------------|---------------------|----------------|-------------------------------|------------------------------|----------------|---------|
| Additive | H ₃ PO ₄ | (| 0.05 M | | vanaulum | Valla | |
| Solvent H ₂ SO ₄ | | 3.8 M | | $(\varphi^0 = 1 \text{ V})^*$ | $ (\varphi^0 = -$ | 0.25 V)* | |
| Seperator/Membra | ne l | Fumasep I | FAP-450 | |] | | |
| Electrode | SIGI | RACELL (| GFD 4.65 E | Ā | VO ₂ + | | 2+ |
| Active Area | | 40 c | m ² | | VO ²⁺ | V ³ | → 3+ |
| | | 5 cycles v | with 1 A | |] | | |
| | | 5 cycles w | /ith 1.5 A | | | | |
| Test Type | | 5 cycles with 2 A | | | | | |
| | | 5 cycles with 2.5 A | | | electrolyte (posolyte) | / electi | rolyte |
| | | 5 cycles v | with 3 A | | | | |
| Parameter | Value | Unit | | F | Parameter | Value | Unit |
| Mean Power | 1.89 | W | | SOC | | 0-1 | |
| Mean Energy content | 2.07 | Wh | | Tank c | ost | 1036 | €/L |
| Current density | 25 | mA/cm ² | | Costs _{ActSpec} | | 2.55 | €/mol |
| A _{Active Area} | 40 | cm ² | | Concentra | | 1.67 | mol/L |
| U _{rev} | 1.25 | V | (| | olvent | 0.07 | €/mol |
| U _{act} | 0.005 | V | | Conce | ntration _{Solvent} | 3.8 | mol/L |
| U _{con} | 0.02 | V | | Costs _A | dditive | 0.44 | €/mol |
| U _{ohm} | 0.05450806025 | V | | Conce | ntration _{Additive} | 0.05 | mol/L |
| | | | | Costs _E | lectrolyte | 155.96 | €/L |

Table 2. Excerpt of essential parameters of the tested 1.67 M vanadium flow batteries.

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| Malarity Active Materi | MV | 0. | 1 M | | A-Hudrovy- | | AV |
|-------------------------|--------|-----------------------|-----|-----|---------------------------------|---------------------------------------|--------------------|
| wolarity Active wateria | TEMPOL | 0. | 1 M | | ТЕМРО | | |
| Additive | NaCl | 1. | 5 M | | $(\varphi^0 = 0.8 \text{ V})^*$ | $ (\varphi^0 = -$ | -0.45 V)* |
| Seperator/Membrane | Fu | Fumasep FAP-450 | | | 4-Hydroxy-2,2,6,6- | 1,1'-Dim | nethyl-4,4'- |
| Electrode | SIGR | SIGRACELL GFD 4.65 EA | | | | Ну | /drat |
| Active Area | | 40 cm ² | | | | MV ² * H ₃ C-*N | N*-сн _а |
| | 5 | 5 cycles with 0.1 A | | | -e- + e- | | -0" + 0" |
| | 5 0 | 5 cycles with 0.25 A | | | 08 | MV** H ₃ C—'N | №_сн₃ |
| Test Type | 5 | 5 cycles with 0.5 A | | | | | |
| | 5 | 5 cycles with 1 A | | | electrolyte (posolyte) | elec (nec | trolyte |
| | 5 | 5 cycles with 1.5 A | | | (peddyte) | | |
| Parameter | Value | Unit | | F | Parameter | Value | Unit |
| Mean Power 0.9 | 98 | W | | SOC | | 0-1 | |

| Mean Power | 0.98 | W |
|--------------------------|---------------|--------------------|
| Mean Energy content | 0.08 | Wh |
| Current density | 25 | mA/cm ² |
| A _{Active Area} | 40 | cm ² |
| U _{rev} | 1.25 | V |
| U _{act} | 0.005 | V |
| U _{con} | 0.02 | V |
| U _{ohm} | 0.05450806025 | V |

| Parameter | Value | Unit |
|-------------------------------------|----------|-------|
| SOC | 0-1 | |
| Tank cost | 1036 | €/L |
| Costs _{ActSpecPos} | 1997.98 | €/mol |
| Concentration _{ActSpecPos} | 0.1 | mol/L |
| Costs _{ActSpecNeg} | 13398.04 | €/mol |
| Concentration _{ActSpecNeg} | 0.1 | mol/L |
| Costs _{Solvent} | 2.17 | €/mol |
| Concentration _{Solvent} | 1.5 | mol/L |
| Costs _{Posolyte} | 403.05 | €/L |
| Costs _{Negolyte} | 1543.05 | €/L |

Table 3 Excerpt of essential parameters of the tested 0.1 M MV/TEMPOL flow batteries.

| | | MV | 0 |). M | | | | | | - |
|--------------------------|--------|-------------------|----------------------|----------------|---------------------|---------------------------------|------------------|--------------------------------------|---------------------|---------------|
| Molarity Active Mat | terial | TEMPOL | | 0.5 M | | 4-Hydroxy- | $\left \right $ | / M | V | , *[<i>I</i> |
| Additive | | NaCl | | 1.5 M | | $(\varphi^0 = 0.8 \text{ V})^*$ | | $(\varphi^0 = -$ | 0.45 V)* | |
| Seperator/Membra | ne | F | umasep | FAP-450 | | 4-Hydroxy-2,2,6,6- | | 1,1'-Dime | thyl-4,4'- | |
| Electrode | | SIGF | RACELLG | FD 4.65 EA | ١ | Tetramethylpiperidin- oxyl | 1- | bipyridiniu Hyd | m-dichlorid Irat | |
| Active Area | | | 40 ci | m ² | | | | MV ^{2*} H ₃ C-*N | N*-сн, | |
| | | 5 | cycles w | ith 0.1 A | | | | - | ·- + | |
| Test Type | | 5 | 5 cycles with 0.25 A | | | | MV** H3C-*N | → → → − сн₃ | | |
| | | 5 | 5 cycles with 0.5 A | | | | | | | |
| | | 5 cycles with 1 A | | | electrolyte | | electr | rolyte |) | |
| | | 5 | cycles w | ith 1.5 A | | (posolyte) | | (nego | siyte) | |
| Parameter | | Value | Unit | 7 | Р | arameter | | Value | Unit | |
| Mean Power | 0.97 | | W | | SOC | | 0-1 | | | |
| Mean Energy content | 0.26 | | Wh | | Tank co | ost | 103 | 36 | €/L | |
| Current density | 25 | | mA/cm ² | | Costs _{Ac} | ctSpecPos | 199 | 97.98 | €/mol | |
| A _{Active Area} | 40 | | cm ² | | Concer | ntration _{ActSpecPos} | 0.5 | | mol/L | |
| U _{rev} | 1.25 | | V | | Costs _{Ac} | ctSpecNeg | 133 | 898.04 | €/mol | |
| U _{act} | 0.00 | 5 | V | | Concer | tration _{ActSpecNeg} | 0.5 | | mol/L | |
| U _{con} | 0.02 | | V | | Costs _{So} | olvent | 2.1 | 7 | €/mol | |
| U _{ohm} | 0.054 | 450806025 | V | | Concer | tration _{Solvent} | 1.5 | | mol/L | |

Table 4 Excerpt of essential parameters of the tested 0.5 M MV/TEMPOL flow batteries.

Costs_{Posolyte}

Costs_{Negolyte}

1080.75

6780.78

€/L

€/L

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The relevant performance parameters for flow batteries are the power density in mW cm⁻² and the energy density in Wh L⁻¹. These are plotted in **Figure 5** against the current densities used in the test series in mA cm⁻².

Figure 5. Plot of the performance data of tested standardized vanadium and MV/TEMPOL laboratory cells with presentation of the mean values and illustration of the standard deviations.

In addition, the voltage, coulomb and energy efficiency of the flow batteries were also determined. In the further course of the project, these can possibly provide information for finding further optimization approaches with regard to the electrolyte selection of flow batteries.

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The voltage efficiency (VE) indicates the ratio of the average discharge voltage to the average charge voltage at constant current. The mean voltages are calculated from the quotient of the integrated area below the charge or discharge curve and the corresponding charge or discharge time (see **Equation** 1). The VE decreases with increasing current density. It is also influenced by a large number of overpotentials such as the diffusion, polarization or ohmic overpotential [6].

Equation 1

Figure 6. Plot of voltage efficiency of tested standardized vanadium and MV/TEMPOL laboratory cells with presentation of the mean values and illustration of the standard deviations.

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The coulomb efficiency (CE) relates the electric charge introduced during the charging process to that recovered in the subsequent discharging process and is calculated according to **Equation** 2. It thus represents an indicator of irreversible side reactions of the redox-active species or electrolyte and cross-contamination between the two half-cell spaces [6].

Figure 7. Plot of coulomb efficiency of tested standardized vanadium and MV/TEMPOL laboratory cells with presentation of the mean values and illustration of the standard deviations.

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Energy efficiency (EE) is a measure of the energy supplied during the charging process that is recovered in the discharging process. It depends in particular on the applied current density and the material quality [6]. The EE is calculated from the quotient of the real energy densities and corresponds to the product of CE and VE (see Equation 3).

$$EE = \eta_C \eta_V = \frac{\overline{E}_{Discharge}}{\overline{E}_{Charge}}$$
 Equation 3

Figure 8. Plot of energy efficiency of tested standardized vanadium and MV/TEMPOL laboratory cells with presentation of the mean values and illustration of the standard deviations.

3.2 Development of the techno-economic model

The hierarchical component model was further developed into a techno-economic model, taking into account the technical and economic data obtained. For this purpose, functions were defined for both areas that represent the mutual dependencies of the individual components in flow batteries of this type.

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3.2.1 Description of the technical dependencies

Technically, these component-wise mutual dependencies can be represented by voltage and resistance, since these are influenced by both Power and Energy.

Under standard conditions, the cell voltage results from the difference of the standard electrode potentials of the cathode and the anode (see **Equation** 4), which in turn corresponds to the potential difference of the respective half cell to the standard hydrogen electrode acting as reference half cell.

$$E^{0} = E^{0}_{Cathode} - E^{0}_{Anode}$$
 Equation 4

The actual reversible cell voltage (U_{rev}) in the de-energized state depends not only on the temperature *T* and the number of electrons *z* converted during the cell reaction, but also on the concentration of the reactants and products of the respective redox reaction. This relationship is quantified by the Nernst equation (**Equation** 5) [8].

$$U_{rev} = (\varphi_c^0 - \varphi_A^0) + \frac{R \cdot T}{z \cdot F} + ln(\frac{c_{C,ox} \cdot c_{A,red}}{c_{C,red} \cdot c_{A,ox}})$$
 Equation 5

R describes the general gas constant, *F* the Faraday constant and c_{ox} or c_{red} the molar concentration of the oxidizing or reducing species.

During the operation of the electrochemical cell, the system is disturbed from its electrochemical equilibrium state and the potentials depend on a variety of other factors such as current density, overpotentials and resistances [5]. The practically measured, i.e. effectively usable, voltage (U_{cell}) between the two electrodes is referred to as the so-called clamping voltage. In this context, reference should also be made here to Ohm's law [9] in equation (**Equation** 6).

U = R I Equation 6

Taking into consideration the mentioned overpotentials, the actual usable cell voltage is as follows:

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$$U_{cell} = U_{rev} - U_{act} - U_{con} - U_{ohm}$$

Equation 7

Where U_{act} represents the activation overpotential, U_{con} the concentration overpotential and U_{ohm} the ohmic overpotential. The latter overpotential can also be represented as the product of the current (I_{cell}) and the inner resistance ($R_{overall}$) using **Equation** 6:

$$U_{ohm} = R_{overall} \cdot I_{cell}$$
 Equation 8

The internal resistance is calculated as the sum of all resistances of the individual components of the cell involved in charge transport:

$$R_{overall} = 2 \cdot R_{current \ collector} + R_{membrane} + 2 \cdot R_{electrode} + Equation 9$$

$$2 \cdot R_{bipolar \ plate} + R_{posolyte} + R_{negolyte} + 2 \cdot R_{carbon \ paper}$$

The resistances of the individual components were generally entered into the technoeconomic model on the basis of the respective material property of the conductivity $(\sigma_{component})$ from the manufacturer's specifications. In addition, the exact areas (A_{active}) and lengths $(b_{component})$ of the laboratory flow battery were used:

$$R_{component} = \frac{b_{component}}{A_{active} \cdot \sigma_{component}}$$
 Equation 10

The number of cells required for the required cell voltage (N_{cell}), which is one of the quantities within the techno-economic model that also has a direct influence on the cost structure, is shown as follows:

$$N_{cell} = \frac{\overline{P}}{I_{stack} \cdot U_{cell}}$$
 Equation 11

This has a significant impact on the cost of the Power section of the FlowBattery.

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The total required electrolyte volume ($V_{electrolytes}$) is decisive for the area of Energy. This is calculated from the sum of the volumes required for the posolyte ($V_{posolyte}$) and the negolyte ($V_{negolyte}$).

$$V_{electrolytes} = V_{posolyte} + V_{negolyte}$$
 Equation 12

These volumes are in turn calculated from the energy content ($W_{electrolyte}$) and the used range of the Status of Charge (SoC_{range}), which is assumed to be 100% for the laboratory flow batteries.

$$V_{electrolyte} = \frac{W_{electrolyte}}{U_{cell} \cdot SoC_{range} \cdot \frac{F \cdot z \cdot c}{3600}}$$
 Equation 13

3.2.2 Description of the economic dependencies

In addition to the technical dependencies, the component-wise dependencies of the costs must also be represented in the techno-economic model. Here, the costs were considered as the sum of the individual costs.

Based on the hierarchical component model (see Fehler! Verweisquelle konnte nicht gefunden werden.), the costs are therefore calculated for the areas of Power (C_{power}), Energy (C_{energy}) and Control & Connect ($C_{control \& connect}$). The total costs of the flow battery (C_{FB}) on a laboratory scale are therefore as follows:

$$C_{FB} = C_{Power} + C_{Energy} + C_{Control \& Connect}$$
 Equation 14

3.2.3 Illustration of the costs for the area of Power (C_{power})

 C_{power} can be broken down again based on the components and also reflects the required number of cells needed to provide the power demanded by the flow battery. In addition, the costs for assembling the cell or, if necessary, several cells into a stack ($C_{final \ stack \ assembling}$) are considered.

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$$C_{power} = C_{current \ collector} + C_{isolation \ plate} + C_{endplate} + C_{connection} + C_{final \ stack \ assembling} + N_{cell} \cdot C_{cell}$$
Equation 15

The cost of the individual cell (C_{cell}) can in turn be represented by the sum of its individual components.

$$C_{cell} = C_{membrane} + C_{electrode} + C_{bipolar \, plate} + C_{gasket \, inside \, cell} + C_{cellframe, \, channel \, \& \, manifold} + C_{screws} + C_{carbon \, paper} + C_{fittings}$$
Equation 16

3.2.4 Mapping of costs for the area of Energy (C_{energy})

The sum of the individual costs of the components in the area of Energy is therefore C_{energy} . The required electrolyte volume (see **Equation** 13) represents the dependence on the required technical performance data of the flow battery. The individual costs result from the individual electrolytes and their tanks.

$$C_{energy} = C_{posolyte tank} + C_{posolyte} + C_{negolyte tank} + C_{negolyte}$$
 Equation 17

The cost of an electrolyte, i.e. the posolyte or the negolyte, is also calculated from the cost of its individual components.

$$C_{electroyte} = C_{active species electrolyte} + C_{solvent electrolyte} + C_{additive electrolyte} + C_{fabrication electrolyte}$$
Equation 18

Specifically, this considers the cost of the active species ($C_{active species electrolyte}$), the solvent ($C_{solvent electrolyte}$), the additive ($C_{additive electrolyte}$) if applicable, and also the cost of manufacturing the entire electrolyte ($C_{fabrication electrolyte}$).

3.2.5 Mapping of costs for the area of Control & Connect (C_{control & connect})

The costs for the area of Control & Connect are not yet linked to the other areas for the FlowBattery at laboratory scale. However, this is conceivable in later investigations for upscaling the model, since the flow rate is coupled with the pump capacity. With

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 $C_{final \ battery \ assembling}$, the costs for the final assembly of the entire flow battery are also considered.

This cost function here is as follows:

 $C_{control \ connect} = C_{pump} + C_{piping} + C_{final \ battery \ assembling}$ Equation 19

By taking all three areas into account, the techno-economic model of a flow battery was finalized on a laboratory scale and adjusted with the aid of the average values determined for the specific test series for the respective electrolyte pairs.

4 Result and discussion

4.1 Distribution of costs

As expected, the distribution of costs differs between the different types of flow batteries (see **Figure 9**). Due to the high level of standardization in the construction of the batteries, the costs in the area of power (C_{power}), i.e. the specific cell, are identical for all flow batteries on a laboratory scale.

For the area of Control & Connect ($C_{control \& connect}$), the costs only vary because during the trials the setup was changed from using a diaphragm pump to using a peristaltic pump, which is significantly more expensive. This change was done with foresight, as it allows the flow rate of the system to be determined more accurately. However, for measuring the current flow battery performance data, this change had no effect other than increasing the cost. Because the pump and other Control & Connect components have no impact on the Energy and Power performance areas in this model, they were also excluded from the cost breakdown in the sensitivity analysis. The value of the total production costs (CAPEX) used there is therefore the sum of the areas of Energy and Power.

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The selection of the electrolyte pair as well as their concentration results in the most visible differences with regard to the total production costs on a laboratory scale. These are decisive for the area of Energy (C_{energy}). Even the reservoirs used for the electrolytes were identical, so changes are always due to the electrolyte pair. The effort required to produce the electrolytes in the laboratory was the same regardless of the electrolyte pair, which is why the estimated costs are also identical. Only for the vanadium electrolyte were such costs not estimated, since this was already purchased ready-mixed (compare **Figure** 10).

Figure 9. Plot of the cost distribution of the total manufacturing costs (CAPEX) of the different flow batteries.

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Figure 10. Plot of the cost distribution of the total manufacturing costs (CAPEX) for the electrolyte pairs of the respective flow batteries.

4.2 Component-wise sensitivity analyses on the techno-economic modell

The techno-economic model was used to perform a wide variety of sensitivity analyses. These can be carried out very well on a component-by-component basis. The results are always prognostic specific costs when varying the studied parameters in the investigated areas. These specific costs are either specific total costs of the energy content in \in Wh⁻¹ or specific total costs of the output in \in W⁻¹.

Methodically, in this investigation it is necessary to keep all parameters constant except for the investigated parameters. Consequently, the results do not represent a real case, since such a variation of one parameter always has effects on almost all other parameters. However, such sensitivity analyses show tendencies which are suitable for making predictions about the system behavior to be expected in principle. In all the investigations carried out, which are discussed in the following subsections, all 3 types of flow batteries showed the same characteristics with respect to the basic behavior. Only the fluctuations with respect to the concrete values were partly different by dimensions

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In the graphs, the actual value of each component examined is marked with a red line. In this way, it is also possible to determine whether there is still a great need for optimization of the component used. In addition to the question of whether an optimal range has already been reached, it is also possible to read how much influence a change has on the specific energy content costs of the flow battery. This influencing variable is subsequently defined as optimization potential (OP). For this purpose, the range of the minimum and maximum values was set in relation to the maximum value (see **Equation** 20).

 $OP_{FB \ energy content, component} = 1 - \frac{specific \ Costs_{FB \ energy content, min}}{specific \ Costs_{FB \ energy content, max}}$

Equation 20

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4.2.1 Effect of current density and active species concentration

Figure 11. Plot of the effect of current density and active species concentration on the specific energy content costs as a quotient of the manufacturing costs (CAPEX) and the energy content of the respective flow battery.

In the sensitivity analysis of current density and active species concetration with regard to the specific energy content costs, an optimum, i.e. the minimum of these specific costs, is not shown at very high or low current densities. Very economical values are already achieved at medium current densities and comparatively low concentrations of the active species. The actual concentration of the active species is shown as a red line for orientation purposes.

Thus, for the vanadium FB, the minimum specific energy content cost of $580 \in Wh^{-1}$ is shown at a current density of 100 mA cm⁻² and 4 mol L⁻¹ concentration of the active species. A similar result of $637 \in Wh^{-1}$ is obtained at a current density of 100 mA cm⁻² and 1 mol L⁻¹ concentration of the active species.

The simulated MV/TEMPOL FB based on the 0.5 M laboratory battery shows the minimum of $5.049 \in Wh^{-1}$ at the current density of 25 mA cm⁻² and 4 mol L⁻¹ concentration of active species. Similar values of $5.083 \in Wh^{-1}$ at the current density of 25 mA cm⁻² and 0.5 mol L⁻¹ concentration of the active species are possible here as well.

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The simulated MV/TEMPOL FB based on the 0.1 M laboratory battery shows the minimum of $15.002 \in Wh^{-1}$ at the same current density and concentration of the active species as the 0.5 M MV/TEMPOL FB. Here, economically comparable operating conditions of $15.207 \in Wh^{-1}$ can be achieved at a current density of 25 mA cm⁻² and 0.3 mol L⁻¹ concentration of the active species.

The significant increase in specific energy content costs at very low and very high current densities can be explained in different ways. When current densities are reduced, the number of stacks needed to provide the required flow battery performance increases exponentially, which significantly increases the cost of the flow battery. A large increase in current density, on the other hand, causes the cost of the required electrolyte to rise sharply, again increasing the cost of the flow battery.

In this sensitivity analysis, the range between maximum and minimum is $44.550 \in Wh^{-1}$ for the vanadium FB, $26.314 \in Wh^{-1}$ for the MV/TEMPOL FB 0.5 M and $63.600 \in Wh^{-1}$ for the MV/TEMPOL FB 0.1 M. This results in optimization potentials of 99 % (vanadium FB), 85 % (MV/TEMPOL FB 0.5 M) and 81 % (MV/TEMPOL FB 0.1 M).

This shows that the optimization of current density and the concentration of the active species is of clear relevance for all flow battery types investigated, which significantly influences the specific energy content costs of the entire battery. Thus, it will always be important to closely match the current densities used in the operation of the flow battery to the electrolyte pairs used in the flow battery and the concentration of their active species. In this way, the economic use of the respective flow battery can be directly influenced.

4.2.2 Effect of effective cell voltage and current density

Figure 12. Plot of the effect of effective cell voltage and current density on the specific energy content costs as a quotient of the manufacturing costs (CAPEX) and the energy content of the respective flow battery.

This sensitivity analysis of effective cell voltage and current density in relation to the specific energy content costs shows almost identical characteristics for all 3 flow battery types. Thus, very economical operating conditions can be achieved even at medium current densities and relatively low effective cell voltages. The actual effective cell voltage of the flow batteries is shown as a red line for orientation.

In the case of the vanadium FB, although the minimum specific energy content cost of $571 \in Wh^{-1}$ is given from a current density of 15 mA cm⁻² and an effective cell voltage of 4 V, similarly economical values of $591 \in Wh^{-1}$ are already achievable at a current density of 50 mA cm⁻² and an effective cell voltage of 1.5 V.

The MV/TEMPOL FB 0.5 M shows its minimum of $4.642 \in Wh^{-1}$ at a current density of 10 mA cm⁻² and an effective cell voltage of 4 V, but similarly economical values of $4.946 \in Wh^{-1}$ are achievable at a current density of 20 mA cm⁻² and an effective cell voltage of 1.5 V.

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The MV/TEMPOL FB 0.5 M has its minimum of $14.832 \in Wh^{-1}$ at a current density of 10 mA cm⁻² and an effective cell voltage of 4 V, but similarly economical values of $15.844 \in Wh^{-1}$ are achievable at a current density of 25 mA cm⁻² and an effective cell voltage of 1 V.

The range between maximum and minimum is $20,800 \in Wh^{-1}$ for the Vanadium FB, $85,800 \in Wh^{-1}$ for the MV/TEMPOL FB 0.5 M and $280,000 \in Wh^{-1}$ for the MV/TEMPOL FB 0.1 M. This results in optimization potentials of 98 % (Vanadium FB), 95 % (MV/TEMPOL FB 0.5 M and 0.1 M).

This shows that the optimization of these factors is of clear relevance for all flow battery types investigated. The optimized operating conditions in terms of effective cell voltage and current density are the essential parameters of all flow batteries investigated. Also, the very high values of the specific energy content costs show the necessity of a good tuning of the investigated parameters especially at low concentrations and comparatively expensive active species of the respective electrolyte pair.

4.2.3 Effect of total inner resistance and current density

Figure 13. Plot of the effect of total inner resistance and current density on the specific energy content costs as a quotient of the manufacturing costs (CAPEX) and the energy content of the respective flow battery.

In the sensitivity analysis of total inner resistance and current density in relation to specific energy content costs, economic operating conditions are more dependent on current density than on total internal resistance. This only has an effect at higher current densities with very high resistances at the same time. The actual total internal resistance of the flow batteries is shown as a red line for orientation purposes.

For the vanadium FB, the minimum specific energy content cost of $598 \in Wh^{-1}$ is given at a current density of 100 mA cm⁻² and a total inner resistance of 0.001 Ω . However, similar economic values of $606 \in Wh^{-1}$ are also achievable at a current density of 100 mA cm⁻² and a total inner resistance of 0.05 Ω .

The MV/TEMPOL FB 0.5 M shows its minimum of $5.056 \in Wh^{-1}$ at a current density of 20 mA cm⁻² and a total inner resistance of 0.001 Ω . Similar economic values of $5.171 \in Wh^{-1}$ are also achievable here at a current density of 25 mA cm⁻² and a total inner resistance of 0.2 Ω .

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The MV/TEMPOL FB 0.1 M has its minimum of $15.597 \in Wh^{-1}$ at a current density of 25 mA cm⁻² and a total inner resistance of 0.001 Ω , but similar economic values of $15.694 \in Wh^{-1}$ at a current density of 25 mA cm⁻² and a total inner resistance of 0.1 Ω .

The range between maximum and minimum is $5,140 \in Wh^{-1}$ for the Vanadium FB, $21,000 \in Wh^{-1}$ for the MV/TEMPOL FB 0.5 M and $68,000 \in Wh^{-1}$ for the MV/TEMPOL FB 0.1 M. This results in optimization potentials of 90 % (Vanadium FB), 81 % (MV/TEMPOL FB 0.5 M) and 82 % (MV/TEMPOL 0.1 M).

Again, optimization of these factors is clearly relevant for all flow battery types studied.

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4.2.4 Effect of weight-specific material costs of active species and effective cell voltage

Figure 14. Plot of the effect of specific material costs of the active species and current density on the specific energy content costs as a quotient of the manufacturing costs (CAPEX) and the energy content of the respective flow battery.

The sensitivity analysis of weight-specific material costs of the active species and the effective cell voltage in relation to the specific energy content costs show that economic operating states are achieved starting at an effective cell voltage of 1 V. At lower cell voltages, economically unfavorable operating states show up comparably quickly. The actual weight-specific costs of the active species and the effective cell voltage are shown as a red line for orientation purposes.

For vanadium FB, the minimum specific energy content cost of $717 \in Wh^{-1}$ is given at an effective cell voltage of 1.8 V and specific material costs of active species of $20 \notin kg^{-1}$. However, similar economic values of $756 \notin Wh^{-1}$ are also achievable at an effective cell voltage of 1.3 V and specific material costs of active species of 10,000 $\notin kg^{-1}$.

The MV/TEMPOL FB 0.5 M shows its minimum of $4.546 \in Wh^{-1}$ at an effective cell voltage of 1.8 V and specific material costs of active species of $20 \in kg^{-1}$. Similar economic values of $4.656 \in Wh^{-1}$ at an effective cell voltage of 1.2 V and specific material costs of active species of $5.000 \in kg^{-1}$ are also achievable here.

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The MV/TEMPOL FB 0.1 M has its minimum of $14.926 \in Wh^{-1}$ at an effective cell voltage of 1.8 V and specific material cost of active species of $20 \notin kg^{-1}$, but similar economic values of $15.350 \notin Wh^{-1}$ at an effective cell voltage of 1 V and specific material cost of active species of $5.000 \notin kg^{-1}$.

The range between maximum and minimum is $2.060 \in Wh^{-1}$ for the Vanadium FB, $8.920 \in Wh^{-1}$ for the MV/TEMPOL FB 0.5 M and 17.700 $\in Wh^{-1}$ for the MV/TEMPOL FB 0.1 M. This results in optimization potentials of 74 % (Vanadium FB), 66 % (MV/TEMPOL FB 0.5 M) and 54 % (MV/TEMPOL 0.1 M).

This shows that optimization of these factors is more relevant for the vanadium FB than for the MV/TEMPOL FB 0.5 M and almost 50 % more than for the MV/TEMPOL FB 0.1 M. The consideration of the electrolytes used show that there is still a slight need for optimization here. Further consideration seems worthwhile.

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4.2.5 Effect of area-specific material costs bipolar plate and conductivity

Figure 15. Plot of the effect of area-specific material costs of the bipolar plate and its conductivity on the specific energy content costs as a quotient of the manufacturing costs (CAPEX) and the energy content of the respective flow battery.

In the sensitivity analysis of the area-specific material costs of the bipolar plate and its conductivity with respect to the specific energy content costs, an optimum, i.e. the minimum of these specific costs, is already shown at comparatively low conductivities, when the specific material costs are also low. The actual area-specific costs of the bipolar plate and its conductivity are each inserted as a red line for orientation.

For example, the vanadium FB shows the minimum specific energy content cost of $728 \in Wh^{-1}$ at a conductivity of 5.200 S m⁻¹ and specific material costs of $20 \in m^{-2}$. However, a similar result of $729 \in Wh^{-1}$ is already shown at the same specific material costs and a conductivity of 20 S m⁻¹.

The simulated MV/TEMPOL FB based on the 0.5 M laboratory battery shows the minimum of $5.067 \in Wh^{-1}$ at a conductivity of 5.200 Sm^{-1} and specific material cost of $20 \notin m^{-2}$. Similar values of $5.103 \notin Wh^{-1}$ at a conductivity of 20 S m⁻¹ and specific material cost of $420 \notin m^{-2}$ are also possible here.

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The simulated MV/TEMPOL FB based on the 0.1 M laboratory battery shows the minimum of $15.596 \in Wh^{-1}$ at a conductivity of 5.200 S m⁻¹ and specific material costs of $20 \in m^{-2}$. Here, economically comparable operating conditions of $15.615 \in Wh^{-1}$ at a conductivity of 200 S m⁻¹ and specific material costs of $140 \in m^{-2}$ can be achieved.

In this sensitivity analysis, the range between maximum and minimum is $4 \in Wh^{-1}$ for the vanadium FB, $37 \in Wh^{-1}$ for the MV/TEMPOL FB 0.5 M and $91 \in Wh^{-1}$ for the MV/TEMPOL FB 0.1 M. This results in optimization potentials of just 0.55 % (vanadium FB), 0.73 % (MV/TEMPOL FB 0.5 M) and 0.058 % (MV/TEMPOL FB 0.1 M).

This shows that for these factors, the optimization potentials are close to zero for all flow battery types investigated. Consequently, optimization of the bipolar plate in terms of conductivity and specific material costs is of negligible relevance when optimizing the respective flow battery.

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4.2.6 Effect of area-specific material costs carbon paper and conductivity

Figure 16. Plot of the effect of weight-specific costs of the carbon paper and its conductivity on the specific energy content costs as a quotient of the manufacturing costs (CAPEX) and the energy content of the respective flow battery.

The sensitivity analysis of area-specific material costs of the carbon paper and its conductivity in relation to the specific energy content costs shows that very economical operating conditions can already be achieved at low conductivities and also low specific material costs. The actual area-specific costs of the carbon paper and its conductivity are inserted as a red line for orientation purposes.

For vanadium FB, the minimum specific energy content cost of $675 \in Wh^{-1}$ is given at a conductivity of 10,000 S m⁻¹ and specific material costs of $50 \in m^{-2}$. Similar economic values of $715 \in Wh^{-1}$ are already achievable at a conductivity of 0.5 S m⁻¹ and specific material costs of 1,000 $\in m^{-2}$.

The MV/TEMPOL FB 0.5 M shows its minimum of $4.860 \in Wh^{-1}$ at a conductivity of 10.000 S m⁻¹ and specific material costs of $50 \in m^{-2}$. Comparably economical values of $5.058 \in Wh^{-1}$ at a conductivity of 0.5 S m⁻¹ and specific material costs of $1.000 \in m^{-2}$ can also be achieved here.

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The MV/TEMPOL FB 0.1 M has its minimum of $14.922 \in Wh^{-1}$ at a conductivity of 10.000 S m⁻¹ and specific material cost of $50 \in m^{-2}$, but similar economic values of $16.243 \in Wh^{-1}$ at a conductivity of 0.5 S m⁻¹ and specific material cost of $2.500 \in m^{-2}$.

The range between maximum and minimum is $2,300 \in Wh^{-1}$ for the Vanadium FB, $10,700 \in Wh^{-1}$ for the MV/TEMPOL FB 0.5 M and $31,800 \in Wh^{-1}$ for the MV/TEMPOL FB 0.1 M. This results in optimization potentials of 77 % (Vanadium FB), 69 % (MV/TEMPOL FB 0.5 M) and 68 % (MV/TEMPOL 0.1 M).

This shows that the optimization of these factors for the flow batteries is comparatively large at about 2/3 to 3/4. However, the material used is already clearly in the economically good range, so that there is no further concrete need for optimization in the laboratory batteries actually built.

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4.2.7 Effect of area-specific material costs electrode and conductivity

In the sensitivity analysis of area-specific material costs of the electrode and its conductivity in relation to the specific energy content costs, economic operating states are already evident at low conductivities above 60 S m⁻¹. The specific material costs of the electrode, on the other hand, have comparatively less effect on the specific energy content costs. The actual area-specific costs of the electrode and its conductivity are inserted as a red line for orientation purposes.

For vanadium FB, the minimum specific energy content cost of $728 \in Wh^{-1}$ is at a conductivity of 1,500 S m⁻¹ and specific material cost of $5 \in m^{-2}$, but similarly economic values of $736 \in Wh^{-1}$ show up already at a conductivity of 50 S m⁻¹ and specific material cost of $500 \in m^{-2}$.

The MV/TEMPOL FB 0.5 M shows its minimum of $5.058 \in Wh^{-1}$ at a conductivity of 10.000 S m⁻¹ and specific material costs of $5 \in m^{-2}$. Similarly economical values of $5.188 \in Wh^{-1}$ can be achieved at a conductivity of 100 S m⁻¹ and specific material costs of $2.500 \in m^{-2}$.

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The MV/TEMPOL FB 0.1 M has its minimum of $15.592 \in Wh^{-1}$ at a conductivity of 10,000 S m⁻¹ and specific material cost of $5 \in m^{-2}$, but similar economic values of $15.724 \in Wh^{-1}$ at a conductivity of 50 S m⁻¹ and specific material cost of $500 \in m^{-2}$.

The range between maximum and minimum is $532 \in Wh^{-1}$ for the vanadium FB, $2,570 \in Wh^{-1}$ for the MV/TEMPOL FB 0.5 M and $7,500 \in Wh^{-1}$ for the MV/TEMPOL FB 0.1 M. This results in optimization potentials of 42 % (vanadium FB), 34 % (MV/TEMPOL FB 0.5 M) and 33 % (MV/TEMPOL 0.1 M).

Consequently, the factors investigated offer optimization potential, but this is of less relevance for all flow battery types studied. In addition, the electrode used is already in economically favorable ranges.

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Vanadium FB 1.67 M MV/TEMPOL FB 0.5 M **MV/TEMPOL FB 0.1 M** FB Costs / € Wh-FB Costs / € Wh-FB Costs / € Wh-1 Range: $| \in \mathbb{Z}^2$ Range: 222 € Wh⁻¹ (~24 %) /€ m² ne / € m⁻ - 6257 1,615 € Wh-1 - 837 - 817 Specific Costs Cost (~24 Specific %) 0.1 Conductivity_{Membrane} / S m⁻¹ Conductivity_{Membrane} / S m⁻¹ Conductivity_{Membrane} / S m⁻¹

4.2.8 Effect of area-specific material costs membrane and conductivity

Figure 18. Plot of the effect of weight-specific effective cell voltage and current density on the specific energy content costs as a quotient of the manufacturing costs (CAPEX) and the energy content of the respective flow battery.

The sensitivity analysis of area-specific material costs of the membrane and its conductivity in relation to the specific energy content costs shows that very economical operating conditions can be achieved even at low conductivities. The specific material costs are clearly of secondary importance. The actual area-specific costs of the membrane and its conductivity are inserted as a red line for orientation purposes.

For vanadium FB, the minimum specific energy content cost of $716 \in Wh^{-1}$ is given at a conductivity of 1.500 S m⁻¹ and specific material costs of $50 \notin m^{-2}$. Similar economic values of $722 \notin Wh^{-1}$ are already achievable at a conductivity of 0.7 S m⁻¹ and specific material costs of 1,000 $\notin m^{-2}$.

The MV/TEMPOL FB 0.5 M shows its minimum of $5.017 \in Wh^{-1}$ at a conductivity of 50 S m⁻¹ and specific material costs of $50 \notin m^{-2}$. Comparably economical values of $5.087 \notin Wh^{-1}$ at a conductivity of 0.5 S m^{-1} and specific material costs of $2.500 \notin m^{-2}$ can also be achieved here.

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The MV/TEMPOL FB 0.1 M has its minimum of $15.447 \in Wh^{-1}$ at a conductivity of 50 S m⁻¹ and specific material cost of $50 \in m^{-2}$, but similar economic values of $15.655 \in Wh^{-1}$ at a conductivity of 0.5 S m⁻¹ and specific material cost of $2.500 \in m^{-2}$.

The range between maximum and minimum is $222 \in Wh^{-1}$ for the vanadium FB, $1.615 \in Wh^{-1}$ for the MV/TEMPOL FB 0.5 M and $5.020 \in Wh^{-1}$ for the MV/TEMPOL FB 0.1 M. This results in optimization potentials of 24 % (vanadium FB), 24 % (MV/TEMPOL FB 0.5 M) and 25 % (MV/TEMPOL 0.1 M).

This shows that the optimization of these factors for the flow batteries is relatively small. Moreover, the material used is already clearly in the economically good range, so that there is no further concrete need for optimization in the laboratory batteries built.

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5 Conclusions and perspectives

The high degree of standardization of a flow battery on a laboratory scale has made it possible to compare different electrolyte pairs as transparently as possible. At the same time, it was possible to develop a techno-economic model on this basis, with which batteries built in this way can be mapped along electrochemical characteristic values with simultaneous evaluation of the economic dimension. Both the technical, i.e. electrochemical parameters, and the economic parameters, i.e. the cost breakdowns, were determined and statistically evaluated in multiple laboratory tests. These validation measurements are also essential in the future in order to investigate further electrolyte pairs in a comparable manner.

The component-specific sensitivity analyses can show which parameters of the components have which techno-economic optimization potentials and also provide an estimate of the scope of the optimizations.

However, the statements of the model cannot yet be applied to flow batteries in medium or large scales, e.g. the application in building or industrial scales. This is primarily due to the fact that the underlying manufacturing costs were initially determined for batteries in the laboratory. Consequently, all component costs are economically distorted and scaling factors or functions must subsequently be found to incorporate the expected economies of scale on a component-by-component basis into the model. This will also significantly increase the strength of the sensitivity analyses.

In addition, the techno-economic model needs to be extended to enable the indicated application up to industrial scales. In some cases, additional components will have to be taken into account in the respective areas. Furthermore, it is foreseeable that additional areas will also have to be considered. For example, the costs of financing and also infrastructure costs will have to be taken into account (see **Figure 19**).

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Figure 19. Hierarchical component model of a larger-scale flow battery, incl. technical and non-technical components.

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This will make it possible to develop a model that is as comprehensive as possible, including existing flow batteries. This will then allow the usual techno-economic forecasts to be made, which will help to find and evaluate techno-economic optimization potentials.

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6 <u>References</u>

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