
DELIVERABLE REPORT

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History			
Date	Version	Partner	Comments
11.12.2023	v0.1	Fraunhofer SCAI	creation
List of Acronyms			
COMPBAT	Computer aided design for next generation flow batteries		
EU	European Union		
FB	Flow Battery		
IEB	Industrial Exploitation Board		
IFBF	International Flow Battery Forum		
IT	Information Technology		
HPC	High Performance Computing		
LIB	Lithium Ion Battery		
SME	Small/Medium Enterprise		
WP	Work Package		

1 General remarks

This document is a report on the in-person workshops carried out to communicate the project's developments and results to the community and to obtain feedback and advice from the experts in practice. Particular attention was paid to the end user group with respect to the functionality and usage of the new workflows and models.

2 Joint Workshop with CompBat at IFBF 2022

In collaboration with the closely related EU project COMPBAT a one-day workshop (Agenda see Table 1) was carried out on 27.06.2022 as a pre-conference event to the annual International Flow Battery Forum. Advertisement and registration took place via the conference website. About 50 persons attended this event from industry and academia (~1:1). At that time (M30/48), the aim was a) to inform the community about the tools and methods under development (morning session) and b) to obtain feedback that could help improve said developments (afternoon session).

Table 1: Agenda of preconference workshop at IFBF in Brussels 2022

09:00 - 09:10	Introduction <i>Speakers: Anthony Price, Jens Noack, Pekka Peljjo</i>
09:10 - 10:30	Technical and industrial collaboration (I) <i>Chaired by Pekka Peljjo</i> <ul style="list-style-type: none">- Screening of FB couples at the atomic/molecular level- Presentations by project participants for Project SONAR
10:45 - 12:30	Technical and industrial collaboration (II) <i>Chaired by Jens Noack</i> <ul style="list-style-type: none">- Assessment of FB opportunities at the cell and system level- Presentations by project participants for Project COMPBAT
13:30 - 14:45	Industrial exploitation <ul style="list-style-type: none">- Discussion of industrial exploitation of EU-funded research
15:00 - 16:00	Panel discussion and general discussion on EC / Industry/research sectors on collaborative research. <ul style="list-style-type: none">- Opportunities for international collaborations
16:00 - 16:45	Poster talks
17:00 - 18:30	Flow Batteries Europe General Assembly (separate registration required)

Thus, special effort was made to obtain feedback from industry with respect to practical and/or research issues and to collaboration options. A prepared chart was handed out among the participants, who were asked to put stickers on those aspects they deemed relevant/critical in their work. The topics were ordered by levels (mainly system, stack, cell, cell components, electrolyte). In addition to the chart, the participants volunteered further information and mentioned other aspects.

Outcome: Across the hierarchy of levels, there was a clear and expectable trend of interest. It ranged from *'new materials'* at the physical component level (electrolyte, electrode, membrane), to *'manufacturing/production'* aspects affecting the central product, to *'management/control'* aspects at the system level. In all these areas, *'design/optimization'* is recognized as a relevant topic, but *'simulations/modelling'* apparently are not considered as the methods of choice to tackle this task.

Although various aspects of *'data management, processing and analyses'* were also offered as an option on the chart, the whole area met with surprisingly little interest, apart from *'standardization'* (of experimental measurements) and experimental measurements for *'digital twins'*. Yet again, there was no connection made to *'simulations/modelling'* as tools in this context.

The participants in the panel discussion were convinced that FBs could become a thoroughly competitive technology for a wide range of applications, yet there was a need to break the momentary vicious circle: no show cases → no demand → low funding → no showcase...

In this circle, different actors/aspects were identified:

Funding situation:

- funding amounts are dramatically below critical mass
- thriving research faces sudden death at the end of a funding period, leading to a loss of knowledge and a breakdown of infrastructure
- applicants for EU projects face great efforts at low prospects, preventing SMEs to commit themselves, even more so, due to the competition between FBs and more advanced technologies.

Scientific challenges:

- for organic electrolytes: demonstrate safety and longevity in a short period of time
- capture the complexity of the technique
 - optimize components and overall behaviour
 - develop battery passport

Market potential:

- + investors realize (in panic) the limits of LIB resources
- + in the long run, FBs are more sustainable than LIBs
- not visible / not comparable to competitors

3 Hands on training at Workshop in St. Augustin 2023

Announced on LinkedIn, Twitter, in the FLORES network and on various conferences (particularly the IFBF in June 2023), the SONAR project members held a one-day workshop on 21/09/2023, including a poster session with presenters' and participants' contributions (Agenda see Table 2). At that time (M45/48), the aim was to inform the community about the project's achievements and the practical usage.

The workshop about modelling techniques and simulation approaches for flow batteries covered all work package topics:

- Computational high-throughput screening
- Atomistic simulation & degradation
- Electrode kinetics, kinetic Monte Carlo & Lattice Boltzmann techniques
- Continuum model-based cell performance simulations
- Pore scale modelling & flow simulations
- Stack & system: coupled physics simulations (electrochemical, hydraulic, thermal)
- Techno-economics

Every subject on the agenda included an introduction into the tools and methods, explanations for the usage and offered the opportunity for questions and answers. For those topics that did not face pragmatic restrictions (e.g., impractically long runtimes and/or licensed code), the users could work with and test pre-installed examples. For that purpose, 20 workstations with internet connection and access to the local HPC cluster were set up and a team of IT staff was always present to help lecturers and participants with any technical problems. The developers themselves guided the users through the exercises and a small tour to visit the local HPC facilities completed the program.

12 participants from outside the SONAR project attended the workshop. It was a mixed audience including students and experts from academia as well as from industry both with/without theoretical or experimental background. They spent a whole day delving deep into the tools and techniques; there was a lively exchange during the workshop.

Table 2: Agenda of hands-on Workshop in St. Augustin 2023

9:00 - 9:10	Welcome	Astrid Maaß
9:10 - 9:30	Introduction	Jens Noack
9:30 - 10:15	Stack & System	Jack Xinjie Guan (remote)
10:15 - 10:40	Pore Scale models I	AmadeusWolf
11:10 - 11:55	Electrode kinetics	Jia Yu, Franco Zanotto (remote)
11:55 - 12:40	Continuum Cell	Roman Schaerer
12:35 - 14:00	Lunchbreak & Site Visit	
14:00 - 14:45	AI & material search	Niklas Dobberstein, A.Maaß
14:45 - 15:30	Ageing & degradation	Xiaotong Zhang
15:30 - 16:15	Holistic	Daniel Gerlach, Ganzorig Davaasuren
16:45 - 17:10	Pore scale models II	Amadeus Wolf
17:10 - 17:30	Feedback & Concluding remarks	Jens Noack, Astrid Maaß
17:30-- open end	Dinner & Poster	

Outcome

The participants appreciated the work done in the project, considered the developed tools as very useful and valued the fact that both experimentalists and simulators were addressed and brought together. The actual instructions needed to execute the simulations, as well as audio recordings of the workshop lectures will be available on the project's website after 31.12.2023.

4 Conclusions

SONAR carried out two workshops, one at half-time, one at the end. While the first one served mainly the purpose to find out what exactly was needed to implement the most useful tools, the second one was intended to inform the community about the actual outcome and to lower the barriers to actually using the software by introducing and explaining it to users in the field. The feedback we received from the community, as well as from the industrial exploitation board was indeed used to guide and finetune the implementations. This led to a very positive reception of the results in the end.