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Enabling Aerospace Electrification by means of Scale-Resolved Battery Simulation

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Abstract. The decarbonization of the civil aviation sector is a challenging task which relies heavily on electrification. Independent of the concept and amount of electrification, e.g. more electric aircrafts (MEA) or even fully electric propulsion systems, the battery plays an important role. The latter are often criticized to be immature in terms of gravimetric energy density. But even if a high-energy cell with a value exceeding 750 Wh/kg on the pack level would be available [1], it is not guaranteed to fulfill corresponding power requirements. Batteries suffer from an energy-power-dilemma and, hence, call for design and optimization of the electrode structure. Inspired by the success of scale-resolved simulations for design and optimization in conventional jet engines, we present a scale-resolved methodology for batteries. The toolbox' potential to increase battery performance is showcased for a Lithium-Sulfur cell. The aforementioned chemistry is broadly anticipated as promising candidate for aerospace applications due to the exceptional high gravimetric energy density.

Introduction

Civil aviation is considered as part of the hard to abate sector [2]. Hence, several parallel technological routes are explored to reach decarbonization and emission goals set by regulatory frameworks [3]. On the commercially established side of the spectrum, optimized combustion-based propulsion is progressed, whereas on the other prospective side of the spectrum electric propulsion is under development.

For the first route it is broadly acknowledged that scale-resolved simulations, i.e. large eddy simulations (LES) [4,5], give invaluable insights to reach the full potential of novel technological adaptions. This concerns immediate short-term improvements through better flow understanding and control, e.g. [6,7], or potential long-term solutions based on sustainable fuels like hydrogen, even requiring a re-design of the injector [8,9]. These recent examples are also supported by the number of R&D codes with industrial relevance available in the community, e.g. AVBP, OpenFOAM, PRECISE-UNS, YALES2 and many more [10].

The second, perspectively more sustainable route of electric propulsion is currently approached by several hybridization concepts that usually involve batteries as key enablers [2,3]. This holds

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independent of the amount of electrification, from more electric aircrafts (MEA) to all electric aircrafts eventually. However, batteries are often criticized in the aerospace context to be immature because of their inherent energy-power-dilemma, i.e. high-energy cells suffer from insufficient power output and vice versa. Considering this battery bottleneck, which physically is an optimization problem of a multiscale reactor somewhat comparable to the traditional combustor, it is indeed surprising that scale-resolved simulations have much lower significance. The only R&D codes we are aware of are BEST/BLIR [11] and 4C [12].

Motivated by this deficiency and the potential to support aerospace electrification, we developed a performant, scale-resolving framework for Lithium-Sulfur batteries based on the open source solver Firedrake [13,14]. The aforementioned batteries are anticipated as a promising candidate for aerospace applications due to the exceptional high gravimetric energy density of 750 Wh/kg on pack level [1]. In [15], the framework was developed for traditional carbon-sulfur (C-S) composite cathodes, which lack significant power capability due to sluggish reaction kinetics. Here, we will show preliminary results for a polymeric cathode material, i.e. sulfurized polyacrylonitrile (SPAN), which eradicates these performance bottlenecks even without optimization measures derived from scale-resolved simulations, holing an untapped optimization potential.

Methods & Results

Our goal is to describe and optimize SPAN pouch cells currently under development in the BMFTR funded project SulForFlight (No. 03XP0491). The current rate performance on pouch cell level is shown and compared in Fig. 1 (a) to a traditional C-S system with similar sulfur loading and an idealized Li-Ion cell of a Boeing 787 MEA [16,17]. Obviously, the overall material system has a large influence on the energy-power-dilemma and the natural question is whether the slope of the SPAN cell, resulting from kinetic limitations at higher currents, can be flattened by structural design.

Therefore, we developed a coarse-grained continuum model (LES-like as in [15]) of the SPAN pouch cell that will be detailed elsewhere. Essentially, it physically describes electric charge and species mass transfer (i) in the SPAN cathode, (ii) in the novel electrolyte system and (iii) at the pristine Lithium anode interface. The developed base reaction scheme from [18] was slightly adapted (Fig. 1 (b)) and eventually, yet consistently, reduced to a one-step reaction

$$\frac{1}{6}\,\mathrm{PAN-S_4-PAN\,(S)} + \mathrm{Li^+\,(L)} + e^-\,\mathrm{(S)} = \frac{1}{3}\,\mathrm{PAN-S-Li\,(S)} + \frac{1}{3}\,\mathrm{Li_2S\,(S)}\,. \qquad (1)$$

This reduction to a one-step scheme allows us to construct a model, which in spirit very similar to usual Li-Ion battery models. The numerical solution is then obtained using Firedrake after discretization with a Discontinuous Galerkin (DG) approach and an implicit Euler time-stepping, which is embedded into a naive feedback controller [15]. Moreover, the resulting coarse-grained continuum model is calibrated by means of a fully homogenized 1D model (red lines) and experimental pouch cell data (grey lines) for discharge profiles as shown in Fig. 1 (c) with a near to perfect match. This is possible under species diffusion dominant scaling conditions [15,19].

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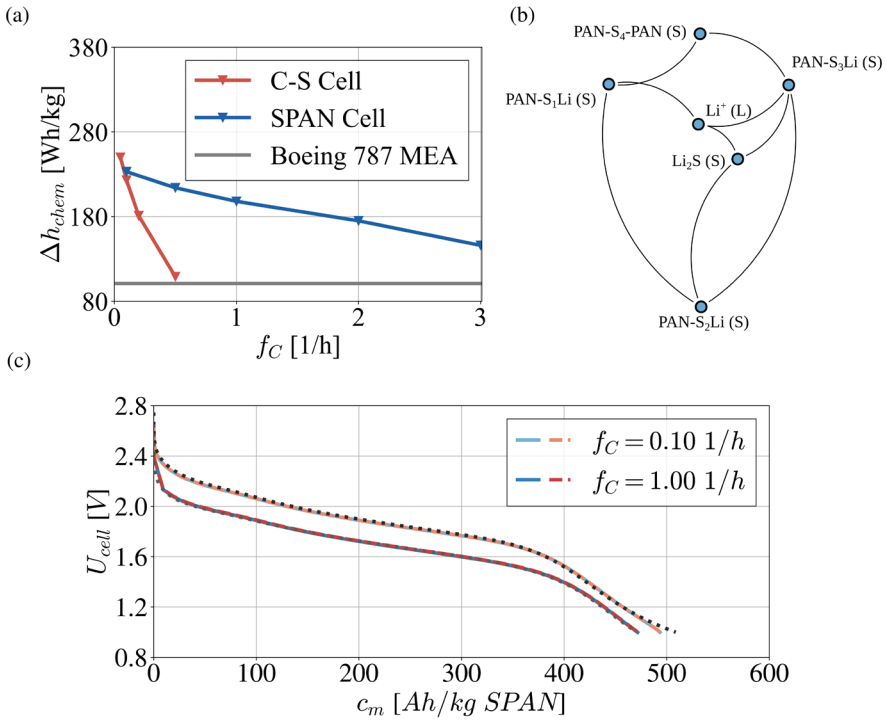


Figure 1: a) Rate performance comparison measured in gravimetric energy density over C-rate, (b) Considered base reaction mechanism for SPAN, (c) Discharge profiles for different C-rates measured in cell potential over discharge capacity.

Based on the resulting parametrization, 3D scale-resolved simulations (blue lines in Fig. 1 (c)) at the same operating conditions were performed. The underlying cathode structure was obtained from a computed tomography (CT) scan with a resolution of 0.6 µm and is highlighted in Fig. 2. The resulting discharge curves verify a posteriori that the assumption of species diffusion dominance on the coarse-graining scale above was justified. This manifests in an expected match of the global characteristics. Naturally, however, it prompts the question why one should perform such costly 3D simulations? A rather intuitive point can be made by looking at the Lithium distribution in the cathode material at the end of discharge (Fig. 2) for a C-rate of $f_C = 1.00\ 1/h$. Even if global characteristics between scale-resolved 3D models and fully homogenized 1D models are identical, the statistical information of inhomogeneous distributions are lost in 1D models by construction. This is not only relevant for degradation phenomena but also the reason why at higher currents, beyond the considered calibration range, fully homogenized 1D models are certain to give wrong predictions as the 3D structure starts to matter [15]. Then, 3D scale-resolved simulations are the only reliable way to tackle the energy-power-dilemma illustrated in Fig. 1 (c). Such simulations are currently a task at hand.

As a final note, we want to shortly comment on the computational cost of the considered 3D model in Fig. 2. Although it comprises only a part of the complete cathode, the emerging discrete problem possesses roughly 110 Mio. degrees of freedom (DoF) and inevitably requires high performance computing (HPC) capabilities. The virtual discharge in Fig. 2 was computed on the bwUniCluster3.0 located at the Scientific Computing Center (SCC) at Karlsruhe Institute of Technology (KIT) using 1536 cores. The virtual discharge took 1.5h, which requires the near to ideal strong scaling behavior of our approach up to 50000 DoF/process [15].

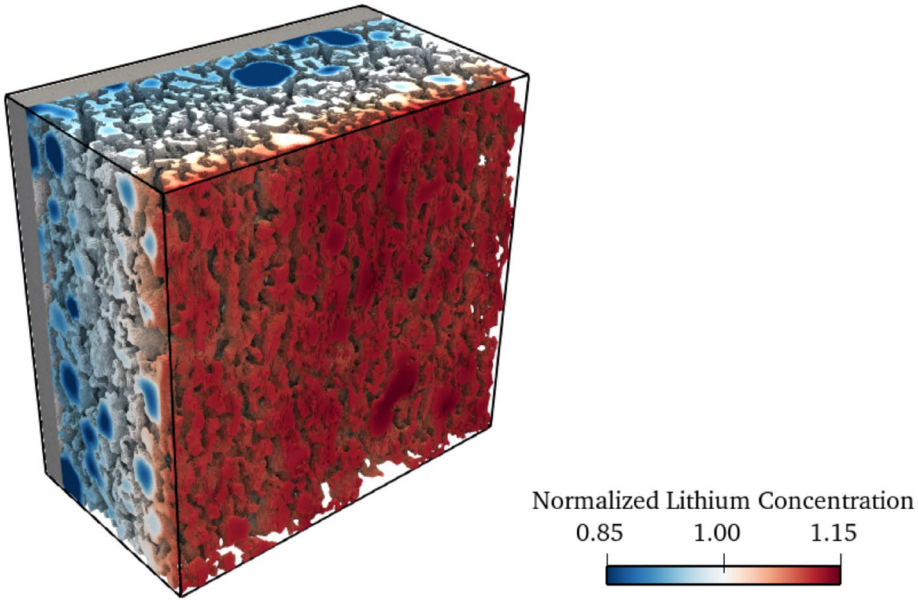


Figure 2: Normalized Lithium distribution in the SPAN cathode structure.

Summary

In this work, we presented preliminary results from scale-resolved simulations of a novel SPAN pouch cell developed in the BMFTR funded project SulForFlight (No. 03XP0491). Therefore, our recently developed 3D scale-resolved framework for Lithium-Sulfur batteries in Firedrake [15] was successfully applied for the first time to a model system similarly used for Lithium-Ion cells. This is as an important step to optimize this polymeric, next-generation Lithium-Sulfur cell in terms of the energy-power-dilemma in Fig. 1 (a). Hopefully, this enables us to tap the full potential of the SPAN cell and contributes to the electrification of the civil aviation sector.

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