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EVALUATION OF MULTIFUNCTIONAL PERFOMANCE IN STRUCTURAL ENERGY STORAGE COMPOSITES USING MULTIPHYSICS MODELING

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ABSTRACT

Multifunctional energy storage composites (MESC) integrate the mechanical properties of composite materials with energy storage devices. This leads to a reduction of the overall system mass with zero weight penalty for energy components such as battery housing. This makes them particularly suitable for applications in the aerospace industry. The two important structural energy storage technologies are structural batteries (SB) and structural supercapacitors (SSC). SBs provide high energy densities, while SSCs have a higher power density. In this study, a digital-based methodology for material selection (called QUINTUS), and another one for design and performance prediction (called FASSEO) for SBs and SSCs are introduced. Based on multiphysics modeling, QUINTUS and FASSEO are able to evaluate the multifunctional performance of SBs and SSCs, and their designs can be optimized, leading to a significantly lower development effort.

1 INTRODUCTION

Multifunctional energy storage composites (MESC) provide structural integrity as well as energy storage capabilities at the same time. MESCs are typically carbon fiber reinforced polymers (CFRP) with integrated batteries or super-capacitors, known as structural batteries (SB) and structural supercapacitors (SSC), respectively (Figure 1). While SBs offer a higher energy density, SSCs provide higher power densities and a better operational safety [1]. Both of these multifunctional materials are currently in the experimental stage and have a low level of Technology Readiness (TRL). Among the challenges are achieving an optimum trade-off between energy density and structural stiffness.

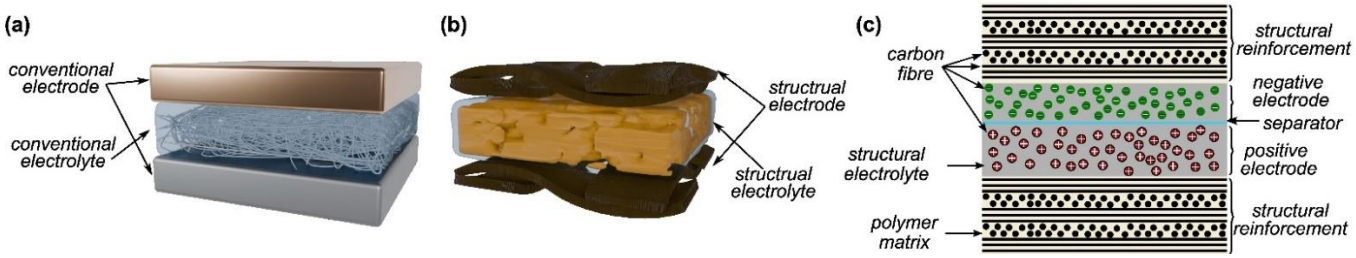

Figure 1. (a) Conventional battery and supercapacitor design, (b) MESC design, and (c) MESC cross-section [2].

Nevertheless, concept studies are available, and demonstrators have been developed for MESCs, such as airplane fuselage components [2], satellite panels [3], and an aerial imaging system [4]. It is anticipated that both SB and SSC will be adopted in lightweight engineering within the aerospace industry in the foreseeable future. Thereby, resource-intensive experimental testing is required to select material combinations and test their performance in candidate applications. Simulation tools based on high-fidelity multiphysics models can reduce such costly

experiments and provide an optimized design for MESCs. Here, two efficient research-based in-house software tools for SB material selection (QUINTUS) and SSC design (FASSEO) are introduced.

2 MATERIALS AND METHODS

The behavior of energy storage devices and composites can be described with physics-based models at single and multiple domains. In the following, these models are briefly reviewed.

2.1 MECHANICAL MODELING

The mechanical modeling of composites at macroscale is typically based on conventional methods for layered materials [5]. For that purpose, shell or layerwise shell methods (Figure 2a) can be used, which are based on approximations such as Classical Laminate Theory (CLT) or First-order Shear Deformation Theory (FSDT) [6]. The CLT assumes that each layer behaves as a homogeneous orthotropic material, while FSDT considers the variation of shear strains through the thickness of the laminate. Alternatively, to account for effects from lower scales, micromechanical modeling approaches can be used. This includes using multiscale homogenization approaches based on representative volume elements (RVE) to transfer specific properties to higher scales [7, 8] (Figure 2b).

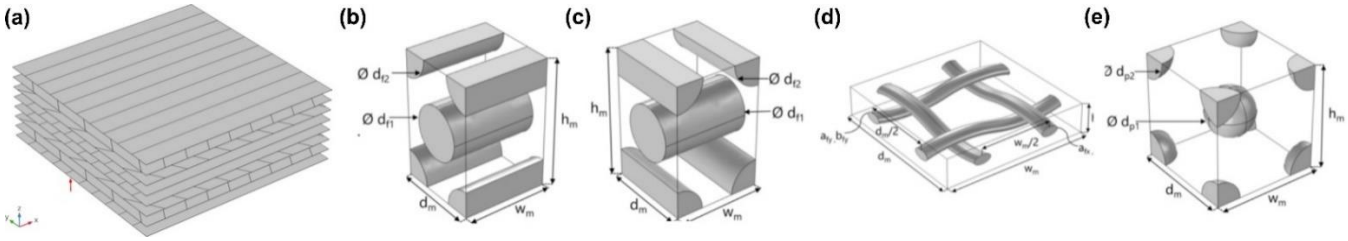

Figure 2. (a) Laminated composite shell, and (b-e) typical RVE geometries [9].

2.2 ELECTROCHEMICAL MODELING

Electrochemical modeling of batteries and supercapacitors can be achieved via two approaches. First is the equivalent circuit method [10], and the second one is the physics-based modeling [11]. The former is a fast approach to monitor the dynamic state of an electrochemical device but it cannot accurately predict the complex electrochemical behavior. Therefore, physics-based models are based on concentrated-solution theories such as Doyler-Fuller-Newman (DFN) [12], the modified single particle model [13], and Poisson-Nernst-Planck (PNP) [14] (Figure 3).

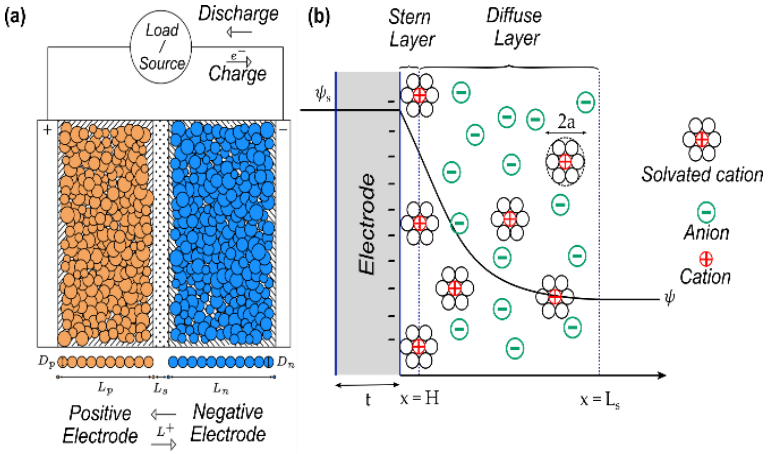

Figure 3. Diagrams of (a) Doyle-Fuller-Newman [12], and (b) Poisson-Nernst-Planck [10] models.

2.3 MULTIPHYSICS MODELING IN MESCS

MESCs are complex materials with multiple functionalities i.e. structural load-bearing capacity and electrochemical energy storage. Charge and discharge behavior of SBs and SCCs have been experimentally proven to be affected by mechanical loads such as compression [15] as well as at elevated temperatures [16] during operation. In other words, various coupled and non-coupled effects take place during MESC operation that need to be understood and predicted [11]. The coupled effects can be one-way (e.g. mechanical-electrochemical coupling in SSCs [11]) or two-way (mechanical-electrochemical coupling in SBs [17]). Multiphysics models use fundamental physics theories involved and capture the interactive effects via dependent variables with direct or indirect couplings [18].

2.4 MULTIFUNCTIONAL PERFORMANCE

According to Ashby's multi-objective optimization approach [19], the unitless multifunctional efficiency of a MESC (η_{mf}) depends on the relative electrical efficiency (η_e) and relative structural efficiency (η_s) [20] and is given as:

$$\eta_{mf} = \eta_e + \eta_s. \tag{1}$$

η_e is defined as the ratio of an overall electro-chemical property, typically energy density, of the MESC concept ($\Gamma_{concept}$) divided by the archived electrical performance of a reference design (Γ_{ref}). Similarly, η_s is defined as the mechanical equivalent in terms of mechanical properties with stiffness ($E_{concept}$, E_{ref}). or strength being widely used, depending on the application case.

$$\eta_e = \frac{\Gamma_{concept}}{\Gamma_{ref}} \text{ and } \eta_s = \frac{E_{concept}}{E_{ref}} \tag{2}$$

3 RESULTS AND DISCUSSION

The multifaceted nature of multifunctional energy storage composites (MESC) presents a formidable challenge in comprehensively accounting for all pertinent effects, particularly when embarking on novel designs from the scratch, encompassing material selection, design concepts, performance prediction, and optimization. To address this complexity, a digital-driven development method is introduced as illustrated in Figure 4, serving as a bridging mechanism across these diverse domains. Leveraging this methodology, two distinct digital frameworks are devised that are tailored for SBs and SSCs, denoted as QUINTUS and FASSEO, respectively. In the following sections, the features of QUINTUS and FASSEO, as well as their respective functionalities and contributions are discussed.

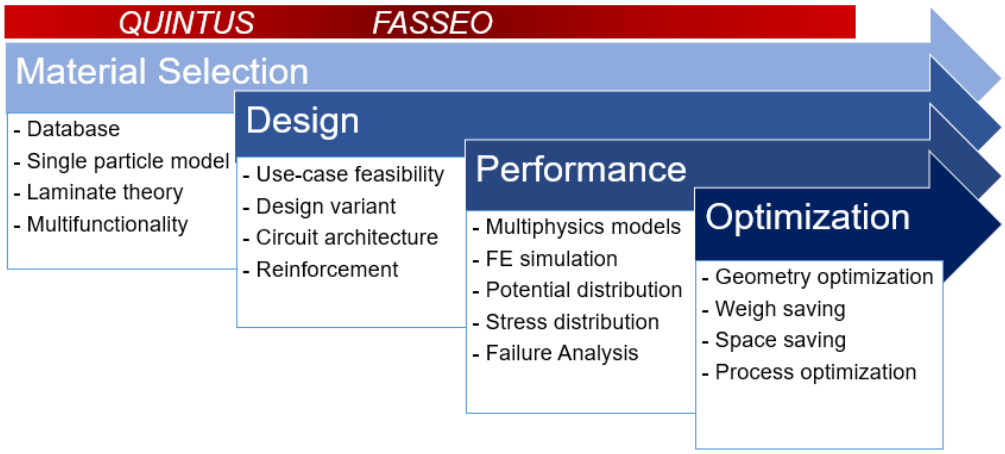

Figure 4. MESC design methodology based on QUINTUS and FASSEO.

3.1 FASSEO

FASSEO, short for Framework for Automated Structural Supercapacitor Engineering and Optimization, is a comprehensive modular tool for SSCs development including design, performance prediction and optimization. The iterative flowchart used in the FASSEO design module is shown in Figure 5a. The module uses concept application input parameters (e.g. composite and battery properties) and SSC data (via experimental results from QUINTUS) to determine whether the design VARIANT is multifunctionally viable (cf. eq. 1). This is accomplished by comparing system requirements (e.g. aerodynamic models in a drone) to the SSC-integrated composite properties. The latter is attained using coupled and uncoupled multiphysics simulation models described in section 2. Should the energy requirements of the SSC design concept be lower than needed (eq. 2), an appropriate circuit architecture is applied to increase total electrical energy. Similarly, additional reinforcement layers are implemented to satisfy structural requirements (eq. 2). In the performance module, input material and process parameters are collected from the user. Processed multiphysics simulation results such as stress distribution and ion concentration in the SSC-integrated geometry are provided as output data using FE solvers in COMSOL Multiphysics. This is done in an intuitive interface which empowers users to make precise performance predictions within a unified framework (Figure 5b). A hallmark feature of FASSEO lies in its ability to facilitate academic and industrial analysis, eliminating the necessity for intricate multiphysics modeling expertise. Furthermore, results from the performance module can be transferred to an optimization module, in which areas for design improvement are identified.

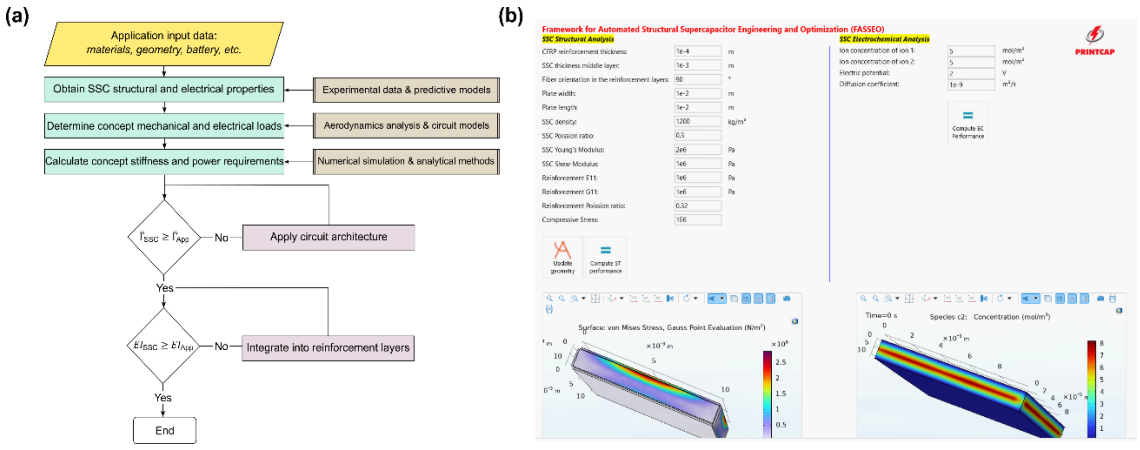

Figure 5. FASSEO (a) design module flowchart, and (b) performance interface (beta-version).

3.2 QUINTUS

Finding suitable materials for FASSEO can be achieved by optimizing the material combinations on a lower scale. This is done via QUINTUS, which is an interface-based modular methodology designed for estimating the properties of composite materials, with a particular focus on battery materials. It leverages a standardized interface framework to streamline data representation and facilitate the registration of multiple models for composite analysis (Figure 6a). The methodology enables the calculation of combined properties such as areal mass and thickness of the battery stack assembly by aggregating the properties of individual components. These properties are crucial for further estimating the electrochemical and mechanical characteristics of the multifunctional composite material. Furthermore, for electrochemical modelling, QUINTUS utilizes an analytical method based on experimentally derived areal capacity and assesses the number of battery cells based on specific sequences. However, more advanced models, such as the modified single particle model to account for electrolyte effects can also incorporated, when required. Mechanical properties, such as Young's moduli of the stack-up are approximated using CLT (see section

2.1). Although finite element method (FEM) based approaches are practical, analytical methods offer comparable results with significantly reduced computational time. QUINTUS prioritizes safety considerations by evaluating different arrangements of anode, cathode, separator, and pouch foil. Lastly, different optimization algorithms, such as a brute force algorithm [21] efficiently generate every conceivable combination. This approach ensures thorough analysis without encountering localization issues or blind spots. This makes QUINTUS a robust tool for composite material analysis (Figure 5b).

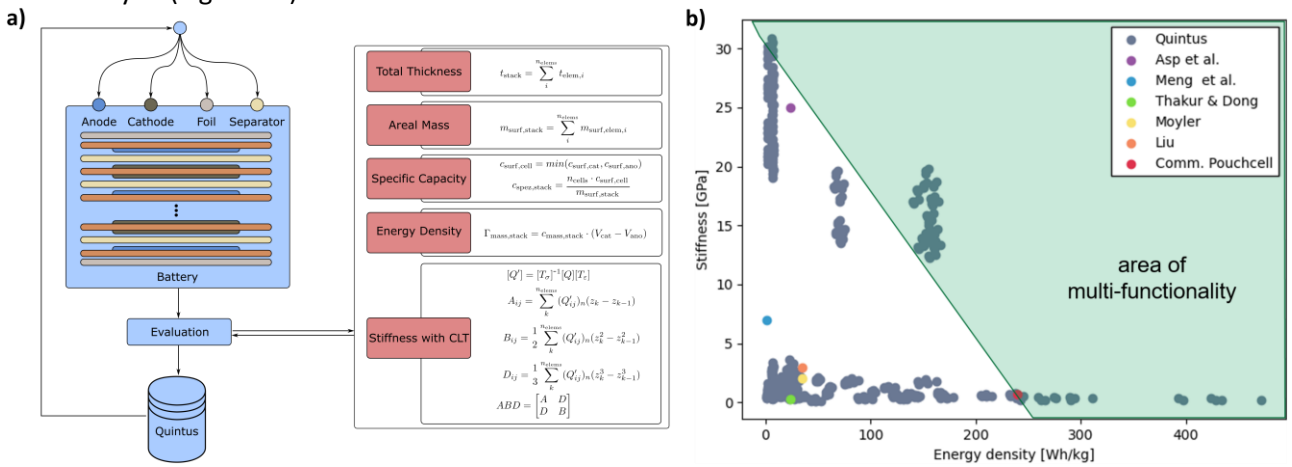

Figure 6. QUINTUS (a) is a modular framework (b) to find better material configurations.

4 Conclusions

Existing constitutive models can be used to predict the performance of composite materials and energy storage devices. However, high-fidelity multiphysics models need to be applied in case of multifunctional energy storage composites. Two digital frameworks, QUINTUS and FASSEO have been developed to accelerate this development at the early design stages. These standalone tools offer insights into material selection, as well as into the mechanical and electrochemical behavior of MESC components under pre-determined mechanical and power loads, without requiring specialized modeling skills. Therefore, QUINTUS and FASSEO are able to minimize the required resources by reducing the number of experimental tests. This will significantly optimize the MESC design and improve properties.

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5 REFERENCES

[1] W. Zschiebsch *et al.,* "Multifunctionality Analysis of Structural Supercapacitors- A Review," *Materials*, early access. doi: 10.3390/ma17030739.

[2] S. Nguyen *et al.,* "Manufacture and characterisation of a structural supercapacitor demonstrator," *Composites Science and Technology*, vol. 245, p. 110339, 2024. doi: 10.1016/j.compscitech.2023.110339. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0266353823004335

[3] J. Petersen, S. Geier, P. Wierach, and M. Wiedemann, "In situ mechanical and electrical characterization of composite-integrated thin film-supercapacitors," *MATEC Web Conf.*, vol. 188, p. 1028, 2018, doi: 10.1051/matecconf/201818801028.

[4] D. Peyrow Hedayati, M. Kucher, H. J. Biggs, and R. Böhm, "Application of structural energy storage devices in aerial monitoring systems: a conceptual design study," in *ICCM 23*, Belfast, Northern Ireland, B. G. Falzon and C. McCarthy, Eds., 2023.

[5] K. M. Liew, Z. Z. Pan, and L. W. Zhang, "An overview of layerwise theories for composite laminates and structures: Development, numerical implementation and application," *Composite Structures*, vol. 216, pp. 240–259, 2019. doi: 10.1016/j.compstruct.2019.02.074. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0263822319300820
[6] N. Nanda and S. Kapuria, "Spectral finite element for wave propagation analysis of laminated composite curved beams using classical and first order shear deformation theories," *Composite Structures*, vol. 132, pp. 310–320, 2015. doi: 10.1016/j.compstruct.2015.04.061. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0263822315003566
[7] J. F. Wang, J. P. Yang, L. Tam, and W. Zhang, "Molecular dynamics-based multiscale nonlinear vibrations of PMMA/CNT composite plates," *MSSP*, vol. 153, p. 107530, 2021, doi: 10.1016/j.ymssp.2020.107530.
[8] K. Lin and Z. Wang, "Multiscale mechanics and molecular dynamics simulations of the durability of fiber-reinforced polymer composites," *Commun Mater*, vol. 4, no. 1, pp. 1–16, 2023. doi: 10.1038/s43246-023-00391-2. [Online]. Available: https://www.nature.com/articles/s43246-023-00391-2
[9] COMSOL AB, *COMSOL Multiphysics®* (2024). Stockholm, Sweden. [Online]. Available: www.comsol.com
[10] D. Peyrow Hedayati, G. Singh, M. Kucher, T. D. Keene, and R. Böhm, "Physicochemical Modeling of Electrochemical Impedance in Solid-State Supercapacitors," *Materials*, early access. doi: 10.3390/ma16031232.
[11] D. Peyrow Hedayati, G. Kahlmeyer, M. Kucher, and R. Böhm, "Numerical simulation of the one-way mechanical-electrochemical coupling in structural supercapacitor," in *Papers and presentations of the COMSOL Conference 2023*, Munich, 2023.
[12] Brady Planden, Katie Lukow, Paul Henshall, Gordana Collier, and Denise Morrey, *A Computationally Informed Realisation Algorithm for Lithium-Ion Batteries Implemented with LiiBRA.jl*, 2022. [Online]. Available: https://www.researchgate.net/publication/359646954_A_Computationally_Informed_Realisation_Algorithm_for_Lithium-Ion_Batteries_Implemented_with_LiiBRAjl
[13] J. Li, N. Lotfi, R. G. Landers, and J. Park, "A Single Particle Model for Lithium-Ion Batteries with Electrolyte and Stress-Enhanced Diffusion Physics," *J. Electrochem. Soc.*, vol. 164, no. 4, A874-A883, 2017. doi: 10.1149/2.1541704jes. [Online]. Available: https://iopscience.iop.org/article/10.1149/2.1541704jes
[14] M. Schmuck and M. Z. Bazant, "Homogenization of the Poisson--Nernst--Planck equations for Ion Transport in Charged Porous Media," *SIAM J. Appl. Math.*, vol. 75, no. 3, pp. 1369–1401, 2015, doi: 10.1137/140968082.
[15] T. Adam *et al.,* "Multifunctional Composites for Future Energy Storage in Aerospace Structures," *Energies*, vol. 11, no. 2, p. 335, 2018. doi: 10.3390/en11020335. [Online]. Available: https://www.mdpi.com/1996-1073/11/2/335
[16] A. Chaichi, G. Venugopalan, R. Devireddy, C. Arges, and M. R. Gartia, "A Solid-State and Flexible Supercapacitor That Operates across a Wide Temperature Range," *ACS Appl. Energy Mater.*, vol. 3, no. 6, pp. 5693–5704, 2020, doi: 10.1021/acsaem.0c00636.
[17] D. Carlstedt, K. Runesson, F. Larsson, J. Xu, and L. E. Asp, "Electro-chemo-mechanically coupled computational modelling of structural batteries," *Multifunct. Mater.*, vol. 3, no. 4, p. 45002, 2020. doi: 10.1088/2399-7532/abc60d. [Online]. Available: https://iopscience.iop.org/article/10.1088/2399-7532/abc60d/meta
[18] J. Xu, G. Lindbergh, and J. Varna, "Multiphysics modeling of mechanical and electrochemical phenomena in structural composites for energy storage: Single carbon fiber micro-battery," *Journal of Reinforced Plastics and Composites*, vol. 37, no. 10, pp. 701–715, 2018, doi: 10.1177/0731684418760207.
[19] M. F. Ashby, "Multi-Objective Optimization in Material Design and Selection," *Acta Metallurgica*, pp. 359–369, 2000.
[20] J. F. Snyder, D. J. O'Brien, and E. D. Wetzel, "Structural Batteries, Capacitors and Supercapacitors," in *Handbook of solid-state batteries* (World Scientific series in materials and energy vol. 6), N. J. Dudney, W. C. West, and J. Nanda, Eds. New Jersey, London, Singapore, Beijing, Shanghai, Hong Kong, Taipei, Chennai, Tokyo: WORLD SCIENTIFIC, 2016, pp. 657–699.
[21] C.-T. Pham and D. Månsson, "Optimal energy storage sizing using equivalent circuit modelling for prosumer applications (Part II)," *Journal of Energy Storage*, vol. 18, pp. 1–15, 2018. doi: 10.1016/j.est.2018.04.015. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S2352152X17305868