CHEMICAL ENGINEERING

FBK - Development and validation of multiphysics-multiscale models and digital twins for redox flow batteries

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Context of the research activity	Research focus will be on the development and the validation of multiphysics-multiscale tools that will accelerate the optimal design and management of redox flow batteries, a technology particularly suited for long-duration energy storage. Flow batteries are a complex system and a multitude of physical phenomena involving different scales (from micro to system) need to be considered to forecast cell and battery system performance and optimize the design of each component.
	Redox flow batteries (RFBs) are a promising technology for large scale energy storage. In RFBs power and energy are decoupled: the former depends mainly on the size of the stack while the latter on the size of the tanks containing the redox active species. This feature makes RFBs ideal for economical, large-scale energy storage. However, cost reductions are mandatory to allow a widespread diffusion of this technology. The required cost reductions involve two main components of the system: the electrolytes and the stack. Both need to be optimized for enabling a large-scale diffusion of RFBs. Flow batteries are complex systems and their design and optimization usually lead to a trade-off between costs and performance (energy and power density, efficiency, cycling life). Cell and stack design is a core task required for the development and upscaling of flow battery systems, but models for redox flow cells can be very complex due to the multitude of physical phenomena that need to be considered: electric fields, fluid flow, mass and species transport in different components, electrochemical reactions, heat transfer. All these phenomena need to be considered for building a digital twin of cell and stack and enable the identification of cell-limiting mechanisms, forecasting the cell performance and optimizing the design. Although some commercial software (e.g., COMSOL) exist to support this activity, they present a lack of flexibility. Moreover, they have serious constraints concerning their use on HPC platforms, as well as their performance, which limits their use to small scale cells. Furthermore, multiscale models that couple detailed cell models and system level models are not currently available.

Objectives	For the above-mentioned reasons, in this PhD project we propose to develop a multiphysics-multiscale platform aimed at supporting redox flow cell and stack design and upscaling. This tool will also enable design optimization supported by different algorithms. The selected candidate will be in charge of developing the models, extending opensource modelling platforms, such as OpenFOAM or FEniCSx and integrating optimization tools such as Dakota. The platform will be composed of different main components tightly connected with each other: 1) Multiphysics cell-scale model. At this scale the electrode will be described as a continuum with transport regulated via permeability and dispersion coefficients obtained from the literature. These are three-dimensional (3D) transient and steady-state simulations characterized by large computational grids, that will require the development of efficient parallelization strategies. If needed some of the model parameters (i.e., permeability and dispersion) can be obtained from geometrically-resolved pore-scale electrode simulations . 2) Stack-scale model. At this scale several cells in parallel will be simulated at once by considering each cell with a simplified description, to highlight possible maldistributions or other issues. This simplified description will be built upon results obtained from cell-scale simulations and will mimic the actual dynamics of the cell. The manifolds of feed and withdraw of liquid solutions will be simulated in its 3D details. 3) System-level redox flow battery model. This model considers the full battery system including the stack, tanks, pumps, piping, power electronics, etc. It is based on transient 1D-0D descriptions (by using OpenModelica or python) that integrates the stack-scale model or a further simplified version. 4) Optimization tool (by using Dakota or python). Optimization can serve two purposes. First, it can be used to calibrate unknown parameters of the 3D cell-scale model by comparing predictions against experimental data. In addition, the optimization tool can be aimed at improving the geometrical cell design to achieve specific targets. If possible, the latter will also be extended to the system-level design by using simplified models. The models and the battery digital twins will be validated with experimental data from known chemistries and representative prototypes and will be then employed to explore new chemistries. The candidate will be responsible for developing and implementing the physical models, validating the models based on experimental data, integrating different models for building a multiscale tool and integrating the optimization algorithms in the workflow to enable design optimization. To enable a strong cross-contamination of ideas and expertise, the candidate might also support the experimental activities related to the validation of redox flow cells with known and new chemistries.

Skills and competencies for the development of the activity	-Strong interest on physics, modelling complex multiphysics transport phenomena and programming -Know-how on electrochemistry and electrochemical devices (batteries, electrolyzers, fuel cells) -Solid know-how on computational methods (e.g., FEM, FVM), experience with opensource tools (e.g., OpenFOAM, FEniCSx) is highly valued -Skills in programming (C++, python) and some experience in the development of applications or libraries for modelling physical systems - Good knowledge of written and spoken English