CHEMICAL ENGINEERING

DISAT - Energy storage systems: multiscale modelling and upscaling

Funded By	Dipartimento DISAT
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Context of the research activity	This Ph.D. project focuses on modeling the charge and discharge process of lithium-ion and sodium-ion batteries to predict their state of health and charge for reliable battery management systems, and to enhance manufacturing and monitoring processes.. The methodologies employed are computational fluid dynamics (CFD) to analyze the effect of electrode composition and structure. Alongside the numerical analysis upscaled models will be developed, using both neural networks as surrogate models, and analytical homogenization techniques.
Objectives	The context of this Ph.D. project is the investigation of electrochemical energy storage systems, especially lithium-ion and sodium-ion batteries. Having robust and accurate models for the prediction of the state of health (which is an indicator of the battery deterioration from its initial specifications) and the state of charge is essential for the construction of reliable battery management systems (BMS) to be used both for safety reasons and performance control. A number of different features have an influence on the performance of a battery during their operation, that is, repeated charge and discharge cycles. Both the chemical composition of the active material and the geometrical structure of this material in the electrode have a huge impact on both the initial behaviour and on the dynamics of the degradation processes leading to performance decreases. The effect of these features is expressed at the microscopic electrode scale (i.e. the scale of the pores) which is hardly explorable experimentally, if at all. For these reasons, numerical computational fluid dynamics (CFD) simulations are envisioned to study the effects of different electrode compositions and geometrical construction. While very accurate, CFD simulations are quite computationally expensive: for these reasons they can be used effectively as tools for optimizing the manufacturing process but they can not be used as fast on-device models providing instantaneous predictions to aid monitoring and control for BMSs. For these reasons, up-scaled models will also be developed based on both numerical and theoretical upscaling techniques, respectively via the construction of neural-network based surrogate models and macroscale

	analytical models obtained with asymptotic two-scale expansion homogenization techniques.

Skills and competencies for the development of the activity	The candidate should have knowledge of transport phenomena and numerical analysis, specifically computational fluid dynamics, along with a working knowledge of coding.