

FC-PAD Characterization Capabilities Used for USCAR Analysis

Partial list of representative FC-PAD capabilities

Techniques	Component	Material Data/Information
SEM/EDAX	MEA	MEA dimensions, composition, structure
TEM – Cross sections	MEA	MEA dimensions, composition, structure, ionomer mapping
TEM – Particle size distributions	MEA	Catalyst particle distribution, size
XRF	MEA	Elemental quantitation
XRF mapping	MEA	Elemental mapping
XCT	MEA	MEA structure
TGA-MS	Catalyst layer	Catalyst wt% / I/C ratio
SAXS	Catalyst	Catalyst particle distribution
EXAFS	Catalyst	Pt-Pt, Pt-Co bonding distances
XRD	Catalyst	Catalyst particle distribution
FTIR	Membrane	Membrane composition
NMR	Membrane/ionomer	Membrane composition/equivalent weight
Titration	Membrane	Membrane equivalent weight
Testing – O ₂ /Air polarization	MEA	Catalyst layer performance
Testing – Catalyst AST	Catalyst	Catalyst durability
Testing – Carbon corrosion AST	Catalyst support	Catalyst support durability
NDIR – Carbon corrosion	Catalyst support	Carbon corrosion measurements
MIP	GDL/MEA	Component porosity
BET	GDL/MEA	Component surface area/pore-size distribution
Contact angle – Sessile drop	GDL/bipolar plate	Component hydrophobicity
Contact resistance	Bipolar plate	Contact resistance
XPS	Bipolar plate	Bipolar plate elemental analysis
XPS – Depth profiling	Bipolar plate	Bipolar plate coating structure
Neutron imaging	Fuel cell stack	In situ water content and distribution during operation

FC-PAD Modeling Capabilities (From FC-PAD's USCAR Collaboration)

Partial list of representative FC-PAD capabilities

Techniques	Component	Information
CL reconstruction from various experimental data (XCT, TEM, PSD, loadings, etc.)	Catalyst layer	Composition and CL microstructure
Direct numerical nano/microscale simulations of gases and liquids	MEA	Detailed distributions and utilization and concentration profiles of critical reactants in individual components (e.g., catalyst agglomerate, GDL fiber domain, CL)
Pore-network simulations	GDL	Examination of multiphase flow using various techniques that accounts for microstructure statistically
Continuum macroscale simulations (voltage loss breakdown and optimization)	Cell and components	Analysis and optimization of cell-level phenomena from 1D to 1+2D models (e.g., CFD) that account for relevant physics including multiphase flow, multiscale phenomena and agglomerates in catalyst layer, non-isothermal, steady-state, or transient. Optimization can also include inverse design and related design rules and metrics.
Multiscale, multi-ion transport in ionomers	Membrane/CL ionomer	Methodology and theories that account for nanoscale phenomena within ionomers up to macroscopic observables. Includes modeling multiple ions (e.g., Ce in membranes)
Multi-model coupling	Various	Methodologies to couple various nano/microscale models (e.g., pore network, direct numerical) with the continuum models
Durability modeling – cell level and voltage loss breakdown	Cell	Transient models of performance that account for changes due to durability concerns MEA structure and ability to analyze performance changes
Membrane degradation	Membrane	Models that examine both chemical and mechanical degradation and related stressors in membranes
Durability modeling – Phenomenon	Various	Specific modeling at the continuum level of degradation mechanisms and durability concerns including start/stop, carbon corrosion, contaminants, etc.
Impedance modeling	Cell, various	Examination of AC and DC impedance results
Data analysis	Various	Algorithms and approaches for data analysis including neural networks
Uncertainty quantification	Various	Analysis of error propagation and uncertainty in data and modeling results including optimization routines and Monte Carlo sampling.