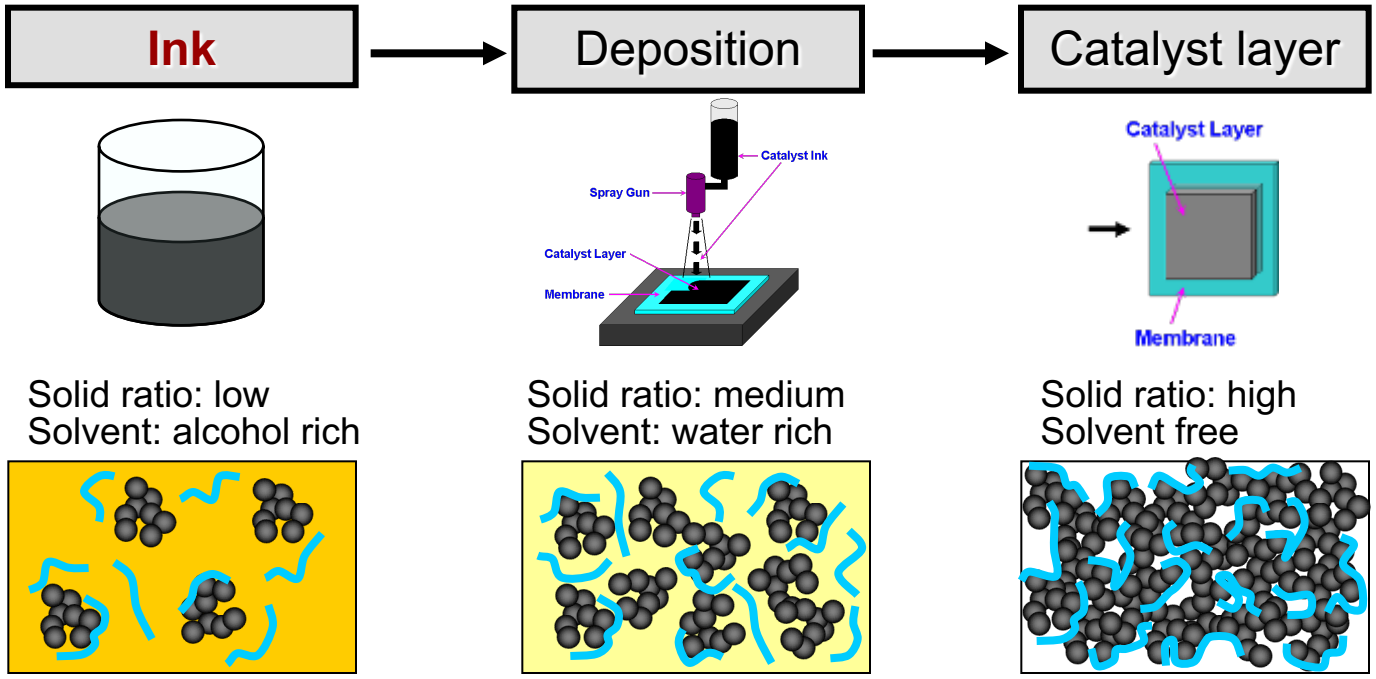
Conventional fabrication process



- Ionomer structure (rod like? adsorbed on C?)
- Carbon structure (aggregated? separated?)
- Structure change during drying process?
- Correlation with transport properties

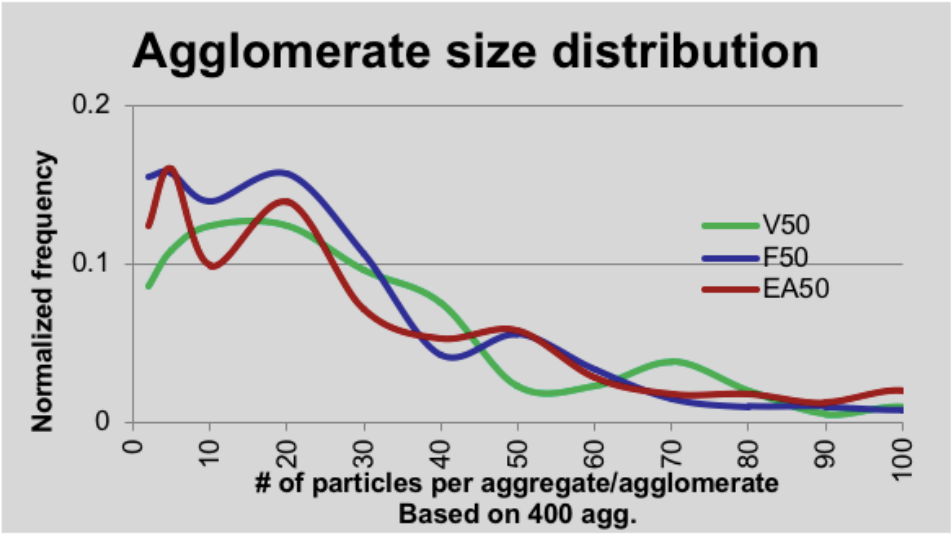
Input (Controllable parameters) → Output

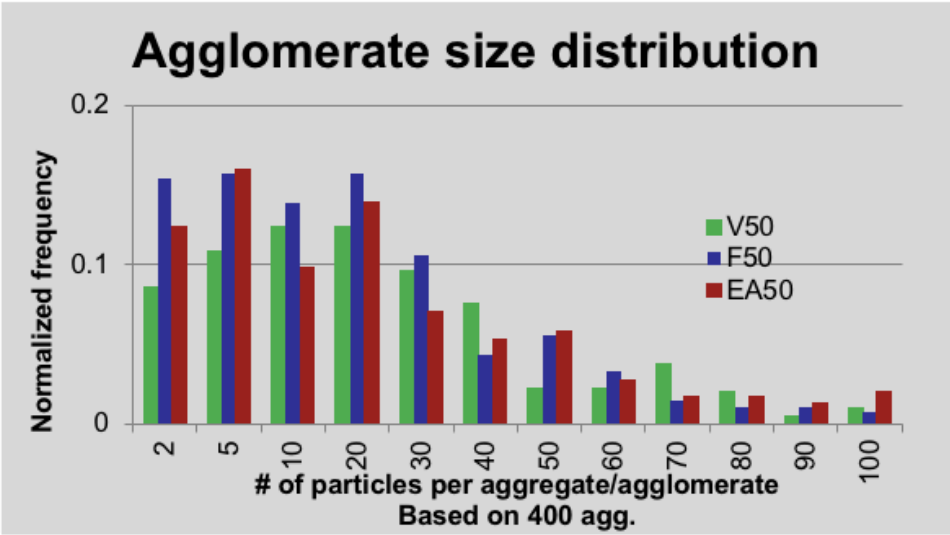
Solvent Ionomer, C, Pt amount	→	Ionomer, C structure in ink (wet phase)	→	Ionomer, C structure in CL (dry phase)	→	Transport properties

NRC-Nissan Collaboration, Internal report

Descriptors at the Ink stage

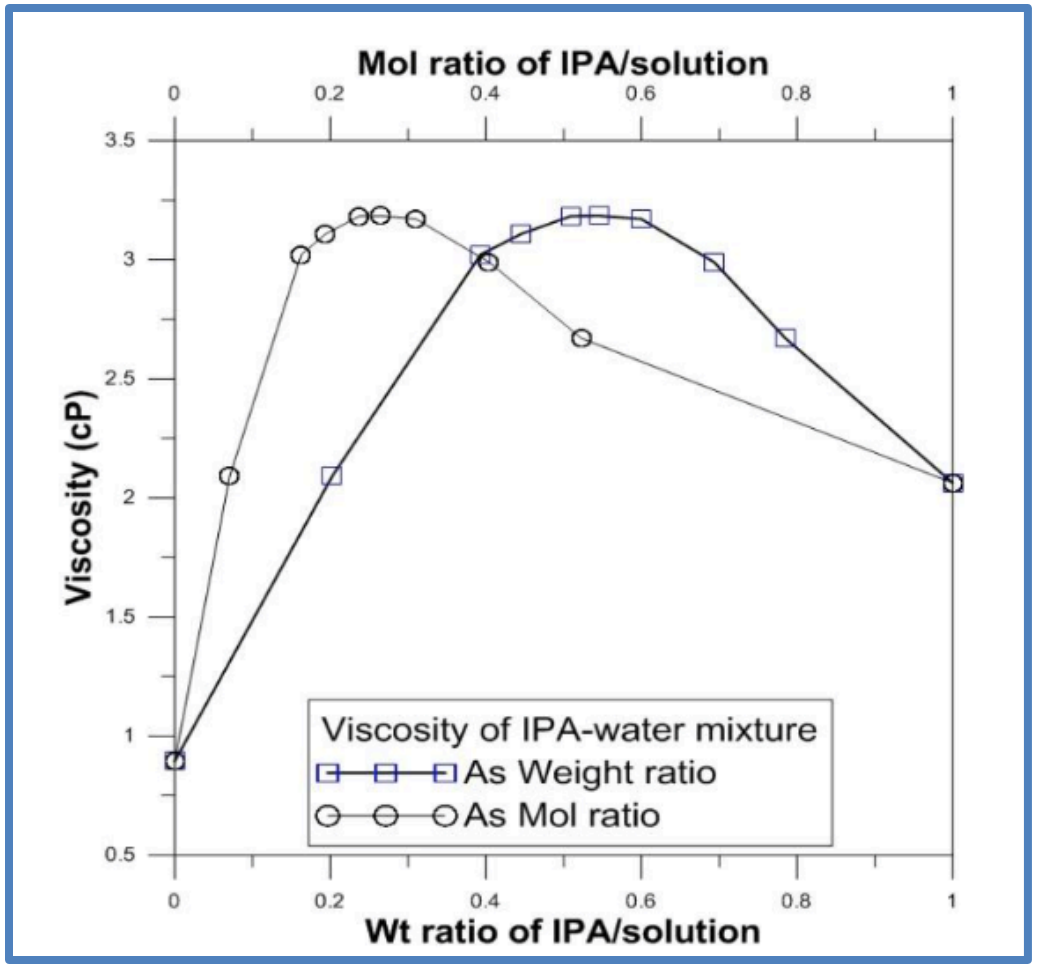
- Viscosity
- Density
- Agglomerate size
- Agglomerate surface area
- # particles /agglomerate
- ….



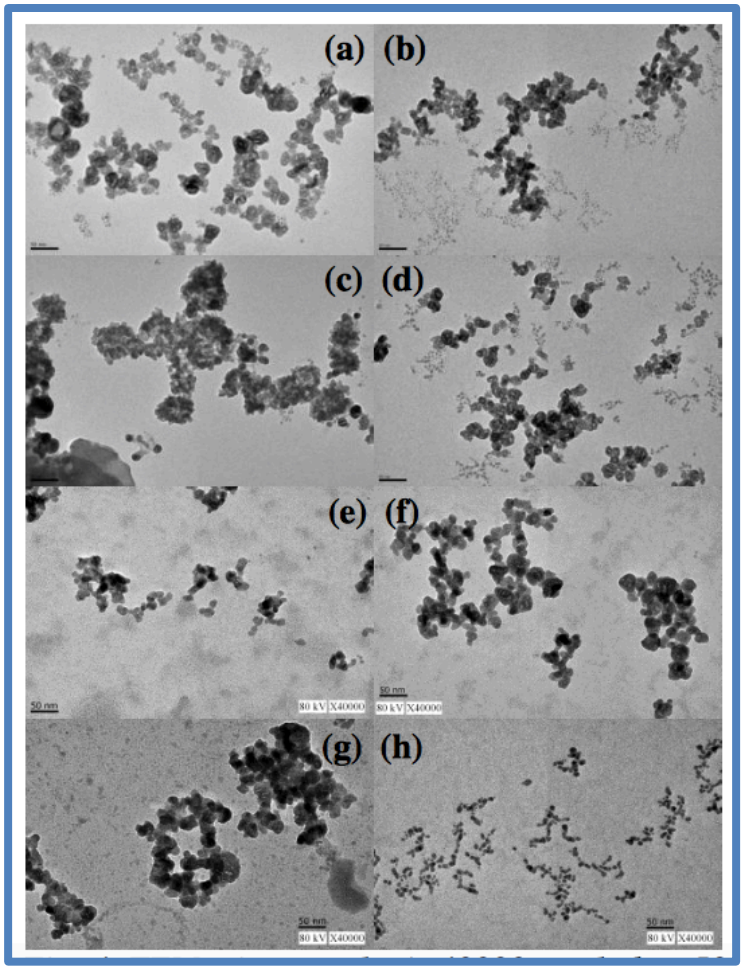


Viscosity

- Modeling / simulation of viscosity?



The concentrations of IPA in the mixture (a) to (h): 20, 45, 50, 55, 60, 70, 80, 100 wt% respectively.

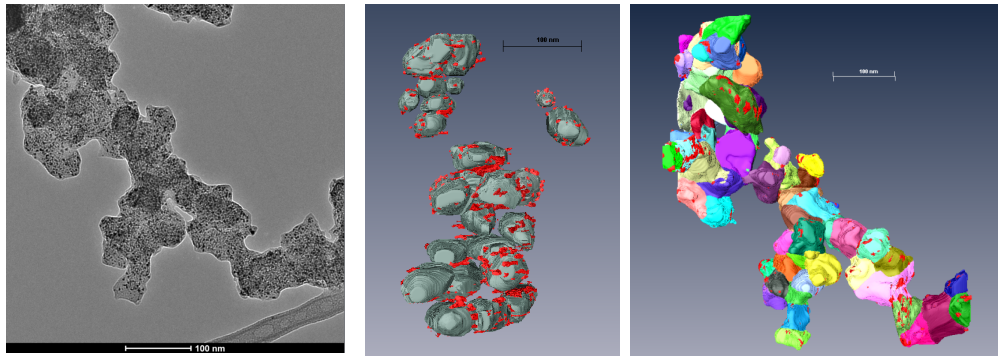


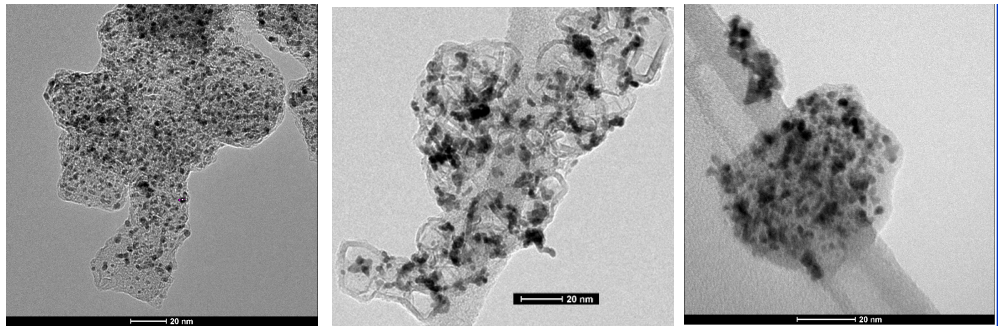
T. T. Ngo *1 , P.S 1 , T. L. Yu
Proceedings of IWNA 2011, November 10-12, 2011

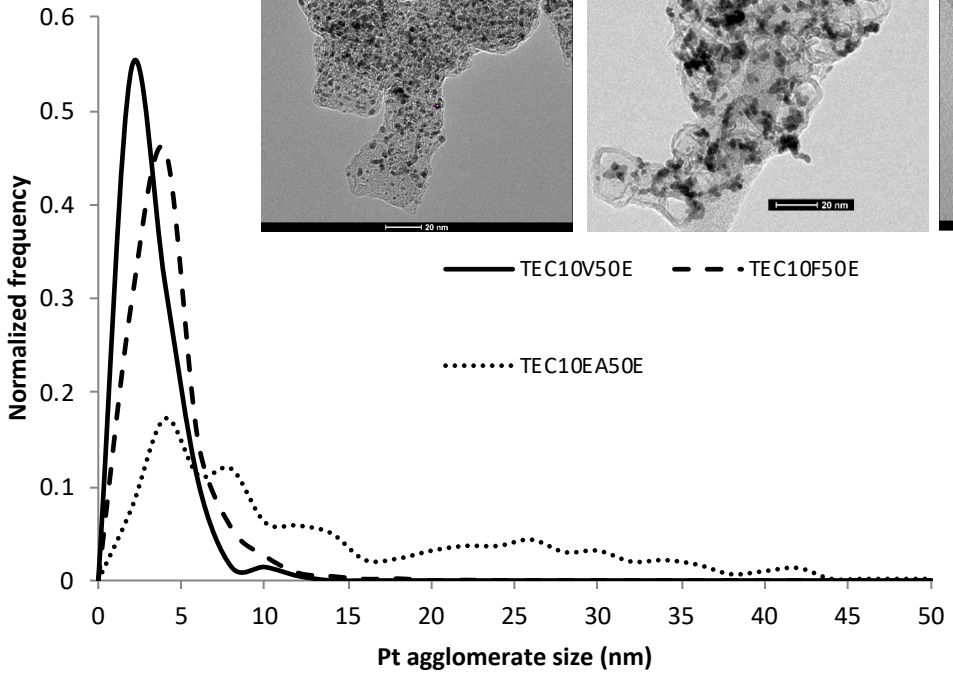
Particle size distribution

3D reconstruction: C support particle size

2D TEM imaging: Pt particle/agglomerate size







Source:
AFCC/Jasna Jankovic (UCON)

Data (MDL/EXP) structure

DFT → AMD → **CGMD** → pore scale model → performance model

design & fabrication — **Cat/Ink-prep.**

characterization — **CCM/MEA-prep.**

validation & testing — **Performance**

Score weighting factor (ML)

Score weighting factor (ML)

Ink								
Level	Category	Parameter	Unit	SOTA	Targets	Target achieved by (year)	Note on the parameter	Target achieved by (year)
Cost	Operating Conditions	Operating Temperature	°C					
		Operating Pressure	Bar					
		Operating current density	kA/m²	1-50	10	2030		
		Cell Voltage	V	1.75	1.5			
		Stack Size	cm²	280				
		Hydrogen purity	%	99.9998				
	Performance							
		Energy Efficiency	%	84				
		Consumed Energy	kWh/Nm3	4.2-7.1				
		Conversion Efficiency (LHV)	%	67				
	Durability							
		Life time	Hour	10,000	10,000-50,000	2020-30		
		Environmental issues						
		Health issues						
		Safety issues						
	Physico-chemical properties	Existing standards and regulations						
	Reliability	Down-time						
		Production cost	$/H2-kg	3.00	<2.70	2017		
Cost	Capital investment	$/H2-kg	0.60	0.30	2017			
	Electrolyzer capital	$/kW	380-480				Stack only	

MEA/CCM								
Level	Category	Parameter	Unit	SOTA (2011)	Targets	Target achieved by (year)	Note on the parameter	Measure/ merit method	Ref.
Cost	Operating Conditions	Operating Temperature	°C	80-100	NA				
		Operating Pressure							
		Operating current density	A/cm²						
		Operating relative humidity	%						
		Cell/stack efficiency	%	34-40	45	2020			
		Transient response (10-90% rated power)	%	85-90	90	2020			
		Start-up time from 20 °C ambient temperature	min	5	2	2020			
	Performance								
		System availability	%	97	99	2020	Percentage of time the system is available for operation (excluding time needed for scheduled maintenance)		
		Operating life time	hr	12,000	60,000	2020	Time until > 20% rel.power degradation. Durability testing should include effects of transient operation, start-up and shutdown		
		Degradation with cycling	%/1000hr	<2	<0.3	2020			
	Durability								
		Environmental issues							
		Health issues							
		Safety issues							
	Reliability	Existing standards and regulations							
		Down-time							
Cost	Equipment cost for 2 kW	US$/kW	NA	2300	1,000	2020	1. Complete system including all necessary components to convert natural gas to electricity suitable for grid connections. 2. Operation on natural gas. 3. Based on 50,000 units/year.		
	Equipment cost for 5 kW	US$/kW	NA	2300	1,500	2020			
	Equipment cost for 10 kW	US$/kW	NA	1,700	<0.3	2020			

Catalyst							Characterization Methods		Additional information		
Priority	Characteristics	Units	2011 status	Targets (2017)	Target (2020)		Established method	Promising early stage tools	Protocol / Ref.	Comment	Known strategy to address technical
	Platinum group total content (both	g/kW (rated)	0.19	0.125	0.125						
	Platinum group metal (pgm) total loading	mg PGM/cm2 electrode area	0.15	0.125	0.125						
	Loss in initial catalytic activity	% mass activity loss	48	<40	<40						
	Electrocatalyst support stability	% mass activity loss	<10	<10	<10						
	Mass activity	A/mg Pt@ 900 mV/iR-free	0.24	0.44	0.44						
	Non-Pt catlayst activity per volume of supported	A/cm3 @ 800 mV(iR free)	(measured at 800	300	300						

MEA						Characterization Methods			
Priority	Characteristics	Units	2011 status	Targets (2017)	Target (2020)	Established method	Promising early stage tools	Protocol / Ref.	C
	Q/ΔT i b	kW°C		1.45	1.45	Q/ΔT i = [Stack power (80kW) x		U.S. DRIVE Partnership/	
	Cost	$ / kW	13 (without frame and gasket)	9	7	Model prediction		Manufacturing Cost Analysis Of Fuel Cell Systems/	Cost
	Durability w/o cycling	Hours	20,000	50,000	100,000	testing/weel established		Partnership/ (http://www.uscar	
	Durability w/o cycling	Hours	12,000	40,000	60,000				
	Performance @ rated power	mW / cm2	845	1000	1000	testing/ weel established protocol		Performance Test Code for Fuel Cell Power	
	Total PGM loadings	mgPGM/cm2	0.19	0.15					
	PGM total content	g/Kw	0.33	0.125					
	mV loss at 0.8 A/cm2	mV	40	<30				30,000 cycles, 0.6-1.0V/ Record #: 11003	
	ECSA loss	%	18					30,000 cycles, 0.6-1.0V	
	mV loss at 1.5 A/cm2	mV	10					1.2 V hold for 400hrs	
	ECSA loss	%	10					1.2 V hold for 400hrs	
	Mass activity loss	%	10					400hrs/ Record	

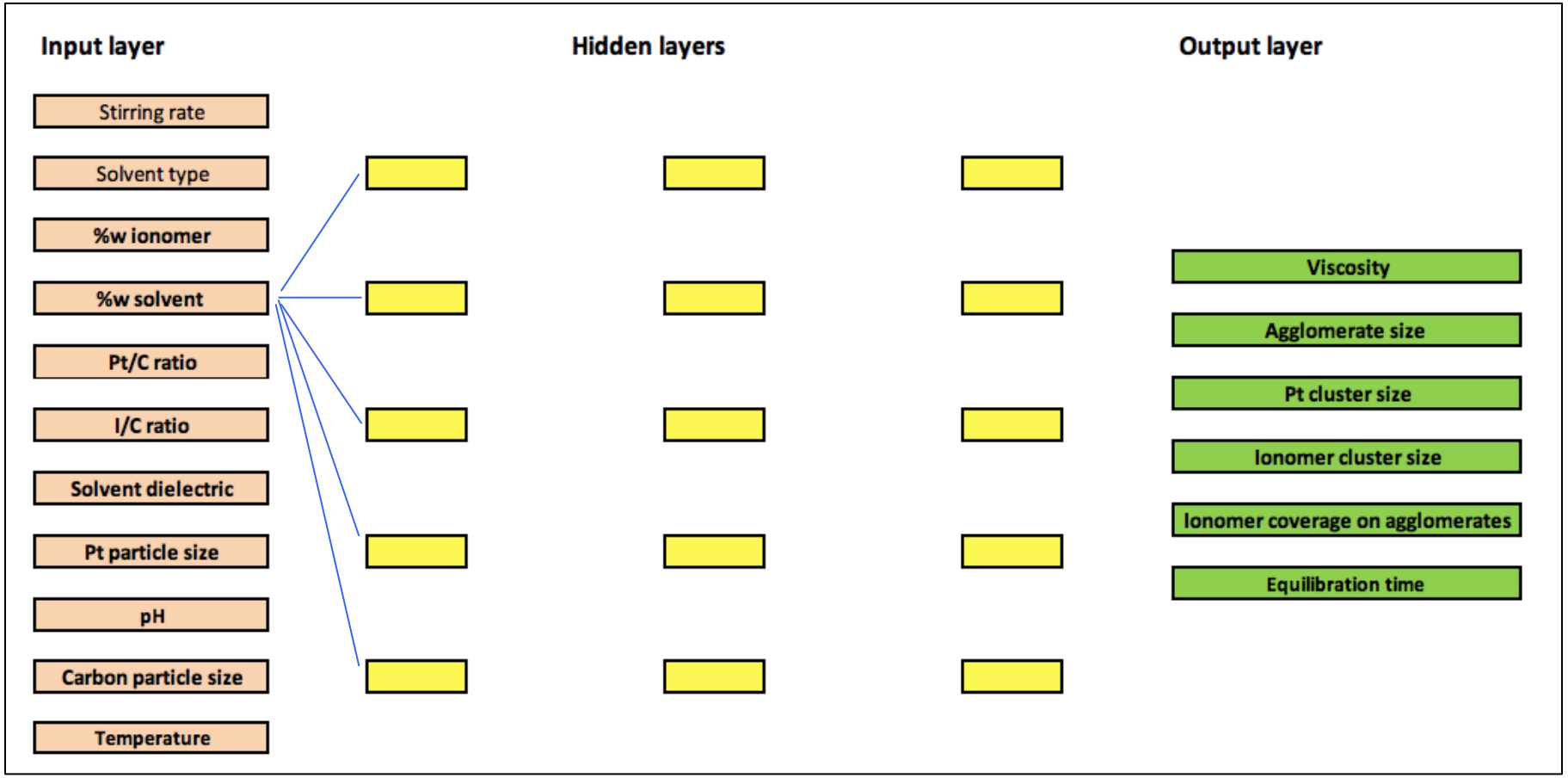
MEA						Characterization Methods			
Priority	Characteristics	Units	2011 status	Targets (2017)	Target (2020)	Established method	Promising early stage tools	Protocol / Ref.	Comment
	Q/ΔT i b	kW°C		1.45	1.45	Q/ΔT i = [Stack power (80kW) x		U.S. DRIVE Partnership/	
	Cost	$ / kW	Y3 (without frame and gasket)	9	7	Model prediction		Manufacturing Cost Analysis Of Fuel Cell Systems/	Costs projected to high volume production (500,000 stack
	Durability w/o cycling	Hours	20,000	50,000	100,000	testing/weel established		Partnership/ (http://www.uscar	40,000 hours durability, 10Kw
	Durability w/o cycling	Hours	12,000	40,000	60,000				fuel cell, for Micro-CHP appl
	Performance @ rated power	mW / cm2	845	1000	1000	testing/ weel established protocol		Performance Test Code for Fuel Cell Power	application. For stationary application, it w
	Total PGM loadings	mgPGM/cm2	0.19	0.15					
	PGM total content	g/Kw	0.33	0.125					
	mV loss at 0.8 A/cm2	mV	40	<30				30,000 cycles, 0.6-1.0V/ Record #: 11003	
	ECSA loss	%	18					30,000 cycles, 0.6-1.0V	
	mV loss at 1.5 A/cm2	mV	10					1.2 V hold for 400hrs	
	ECSA loss	%	10					1.2 V hold for 400hrs	
	Mass activity loss	%	10					400hrs/ Record	

MEA/CCM								
Level	Category	Parameter	Unit	SOTA (2011)	Targets	Target achieved by (year)	Note on the parameter	Measure/ merit method	Ref.
Cost	Operating Conditions	Operating Temperature	°C	80-100	NA				
		Operating Pressure							
		Operating current density	A/cm²						
		Operating relative humidity	%						
		Cell/stack efficiency	%	34-40	45	2020			
		ChP efficiency	%	85-90	90	2020			
		Transient response (10-90% rated power)	%						
		Start-up time from 20 °C ambient temperature	min	5	2	2020			
	Performance								
		System availability	%	97	99	2020	Percentage of time the system is available for operation (excluding time needed for scheduled maintenance)		
		Operating life time	hr	12,000	60,000	2020	Time until > 20% rel.power degradation. Durability testing should include effects of transient operation, start-up and shutdown		
		Degradation with cycling	%/1000hr	<2	<0.3	2020			
	Durability								
		Environmental issues							
		Health issues							
		Safety issues							
	Reliability	Existing standards and regulations							
		Down-time							
Cost	Equipment cost for 2 kW	US$/kW	NA	2300	1,000	2020	1. Complete system including all necessary components to convert natural gas to electricity suitable for grid connections. 2. Operation on natural gas. 3. Based on 50,000 units/year.		
	Equipment cost for 5 kW	US$/kW	NA	2300	1,500	2020			
	Equipment cost for 10 kW	US$/kW	NA	1,700	<0.3	2020			

Deep Neural Network

Collaboration:

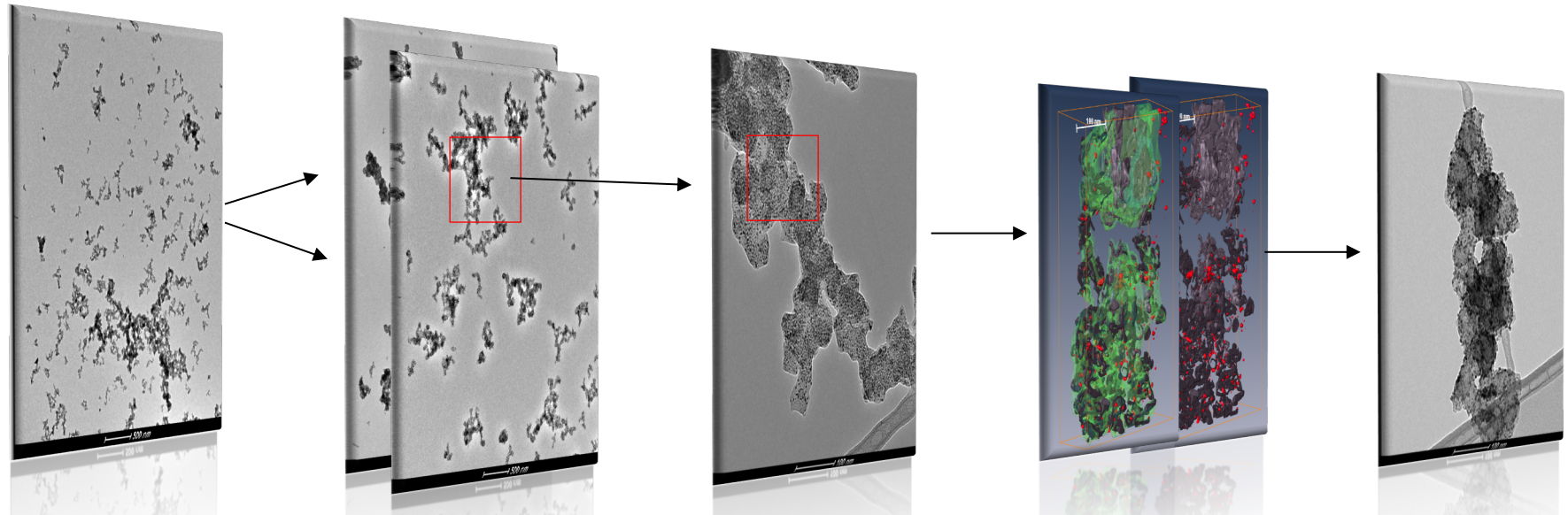
- Jenia Jitsev (JSC)



Convolutional Neural Network

Collaboration:

- Jenia Jitsev (JSC)
- Jasna Jankovic (UCON)



Example of Data Structure

Category	Technical parameters	Unit	SOTA
Performance	HER specific activity @ ?V vs RHE (Reversible Hydrogen Electrode) potential, P kPa, T°C.	A/cm^2 - Pt	
	Mass activity @ 1.65 V or less and should be a half cell measurement; doesn't ft with method proposed	mA/mg	
Performance	Tafel slope	mV/dec	60
Cost	Total cathode PGM loading	mg/cm$^2_{planar}$	0.15 - 0.3
	wt% PGM-on-support	wt%	100
Durability	Degradation rate under some type of accelerated stress test of X,000 cycles	mV/cycle	reported negligible in current experiment being conducted.
Physical properties	Catalyst particle diameter	nm	3-10
Physical properties	Pt/PGM morphology	-	semi-spherical
Physical properties	Specific surface area (NSTF)	m^2/g	~ 10
Physical properties	Specific surface area	m^2/g	900-1000
Physical properties	Catalyst support Electornic conductivity	S/cm	>0.01
Physical properties	Exchange current density	mA/cm2	10^-6
Cost	Manufacturing cost @ x volume	$/unit @ x volume	company sensitive
	Selling price @ x volume	$/unit @ x volume	