

Heat and mass transport phenomena in polymer electrolyte membrane fuel cells micro/nano porous layers

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Polymer Electrolyte Membrane Fuel Cells

Objective:

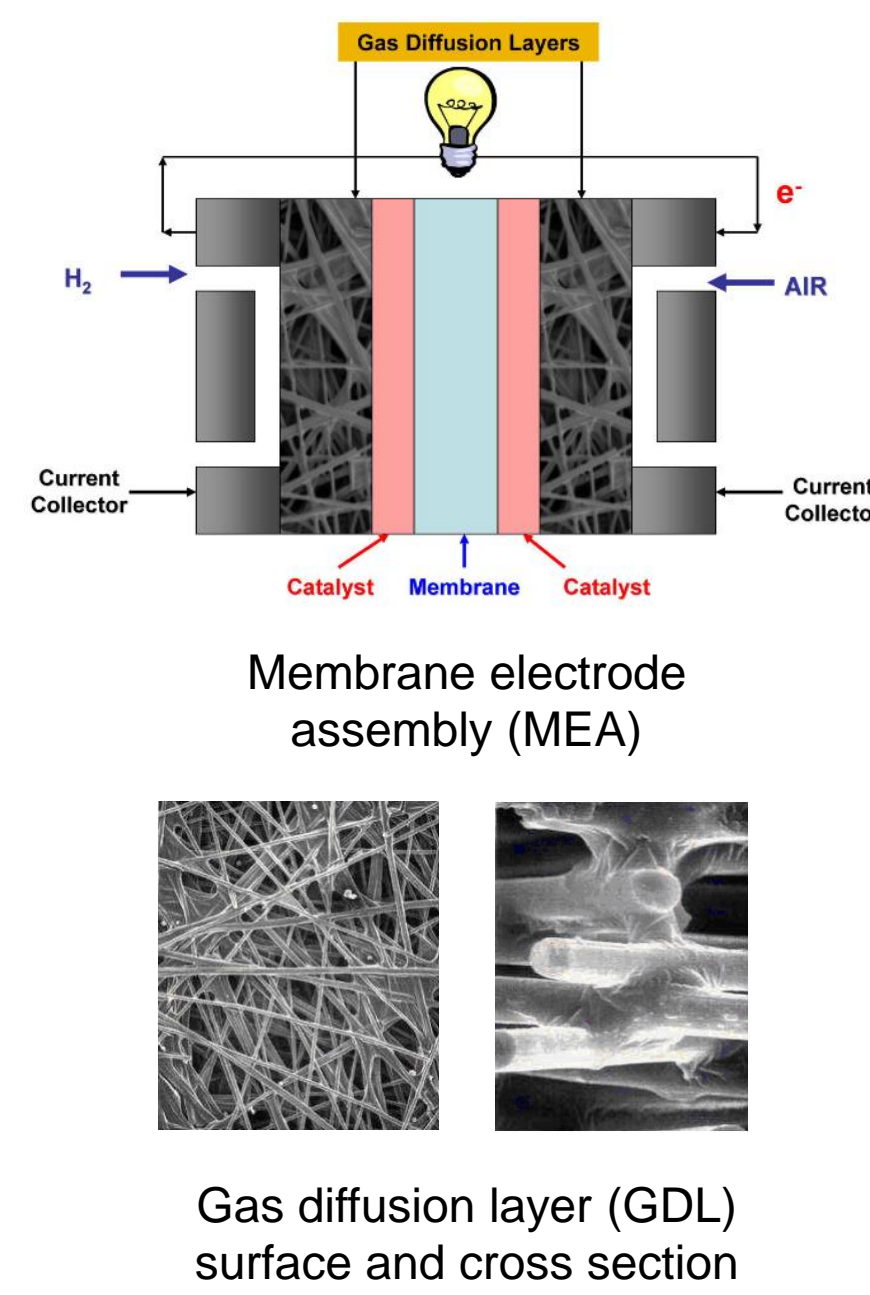
Perform cutting-edge research on PEM fuel cell materials focused on analytical modeling and experimental investigation of the transport properties of micro/nano structured fuel cell components, including:

- Thermal conductivity
- Diffusivity
- Permeability
- Interfacial resistance
- Electrical conductivity

The performance of a PEMFC relies on the effectiveness of the transport of heat, mass, and charge in membrane-electrode assembly (MEA)

Diffusion is the mechanism through which gas of reactants reach Pt nanoparticles in catalyst layer (CL)

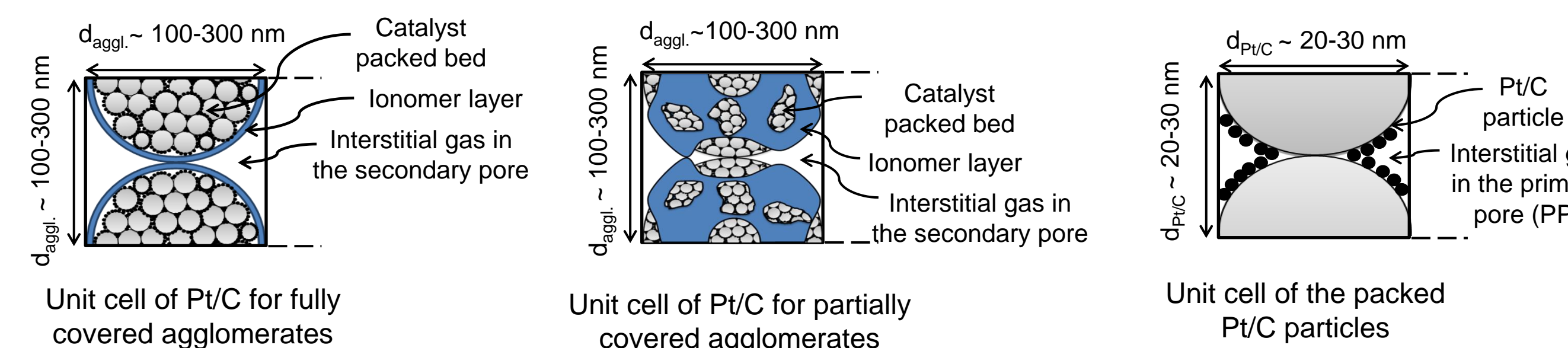
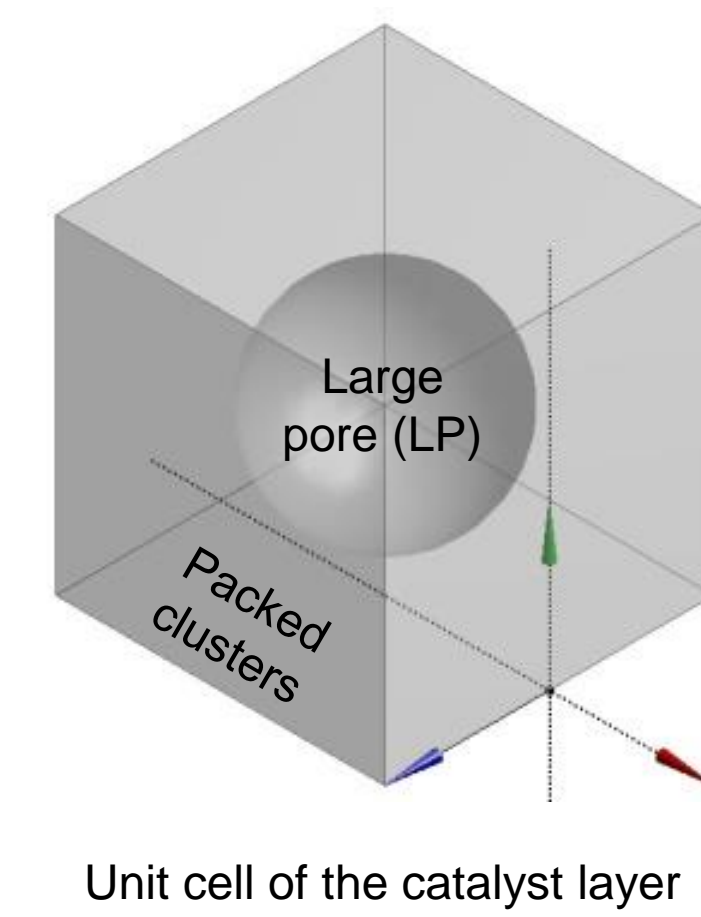
The better design of the CL, the more active Pt nanoparticles, the less Pt loading required in CL, and the lower the production cost



Heat Transfer Model for Catalyst Layer

Modeling by a multi-scale unit cell approach:

- Unit cell of the catalyst layer at micro-scale
- Unit cell of the agglomerates clustered around pores at nano-scale
 - Agglomerates fully covered by ionomer
 - Agglomerates partially covered by ionomer
- Unit cell of carbon supported platinum particles (Pt/C) inside each agglomerate at nano-scale
- Fundamental heat transfer and elasticity laws are used to model the local properties and transport phenomena within each unit cell
- The unit cell models at multiple scales are integrated to obtain the heat transfer model of the whole catalyst layer

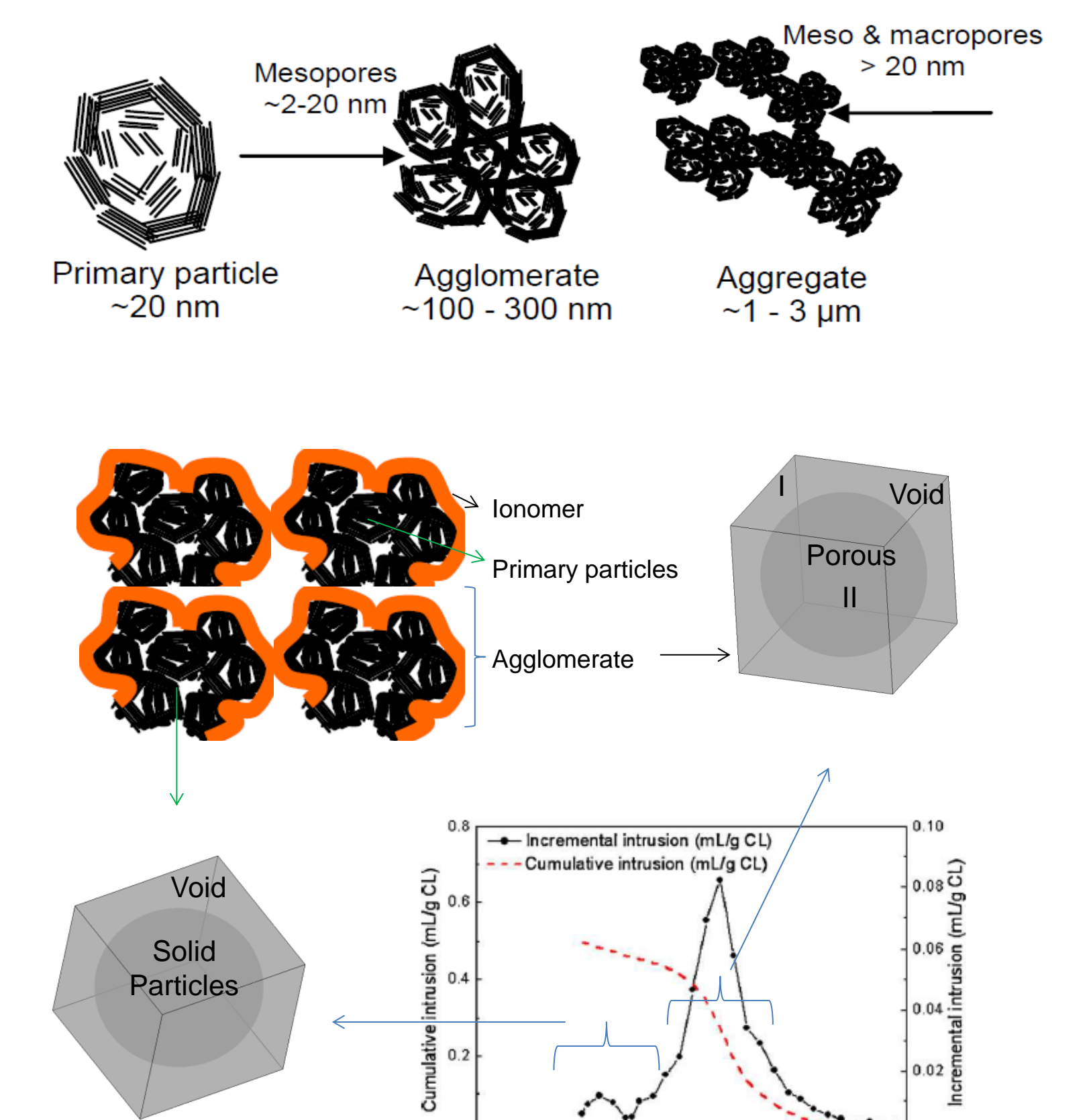


Modeling the effect of ionomer coverage

Diffusivity Model for Catalyst Layer

Different unit cells for pores with different equivalent diameters

- Unit cell around primary particles consist of solid and void parts ($D < 50$ nm)
- Unit cell around agglomerates consist of porous and void parts ($50 \text{ nm} < D < 300 \text{ nm}$)
- Unit cell around aggregates consist of porous and void parts ($300 \text{ nm} < D < 3 \mu\text{m}$)
- Considering both Knudsen and bulk diffusion mechanisms
- Considering temperature dependency



Future work

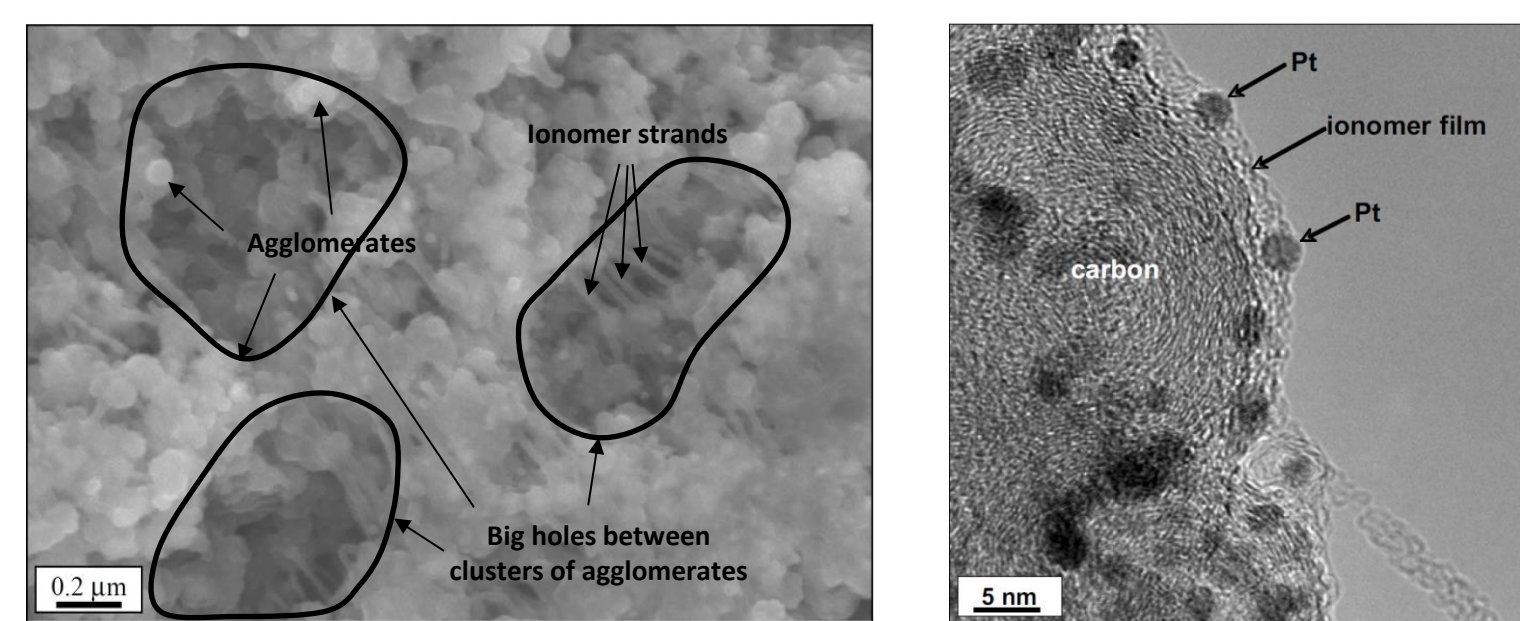
- Ionomer coverage
- Humidity
- Compression
- More realistic unit cell geometry

Platinum Catalyst Layer

Carbon supported Platinum (Pt/C)

In the catalyst layer, platinum nanoparticles are supported by carbon black particles which aggregate into agglomerates.

The agglomerates are connected by ionomer and reactant gases flow through pores in the layers.



SEM (left) and TEM (right) images of the ionomer strands that bind Pt/C agglomerates together and the microstructure of Pt/C/ionomer at the surface of an agglomerate.

More, K.L., et al., ECS Transactions, 3(1), p. 717 (2006)

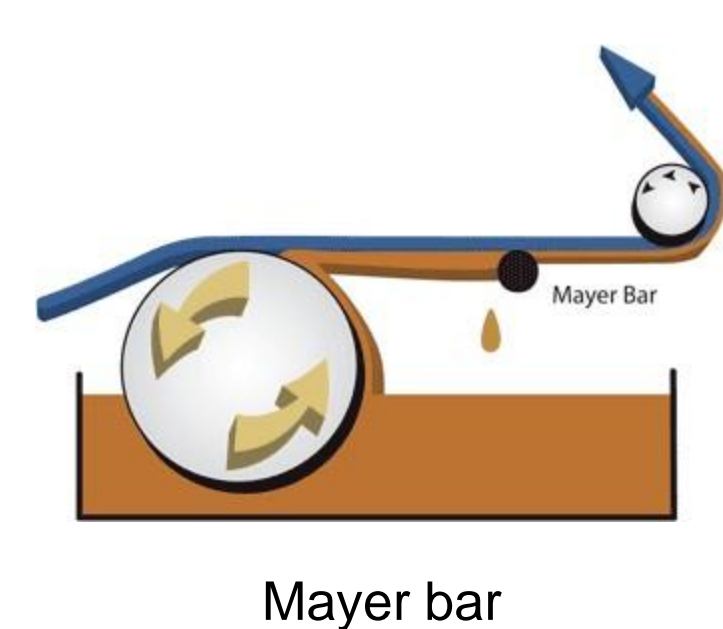
Catalyst layer preparation

Ink preparation:

- Mixing of Pt/C, ionomer and solvents
- Probe sonication of mixture
- Magnetic stirring

Layer deposition on membrane:

- Fuji inkjet printer and Microfab printer
 - Good for small areas
 - Printing thin layers of catalyst
- Mayer bar rolling transfer
 - Good for mass production
 - Coating thick layers of catalyst



Fuji inkjet printer

Characterization:

- Scanning electron microscopy of epoxy mounted cross-sections to evaluate layer thickness
- N_2 adsorption porosimetry to evaluate pore size distribution and porosity
- FIB-SEM to study the structure of catalyst layer



In 2008, Ballard, Ford and Daimler formed the Automotive Fuel Cell Cooperation Corporation (AFCC). The LAEC-AFCO collaborative research project on transport phenomena in fuel cell porous layers began in May 2014.

Sources of waste heat generation in a PEMFC:

- Reversible heat of the electrochemical reaction (in CL)
- Irreversible heat due to activation losses (in CL)
- Latent heat due to phase change (in cathode CL)
- Joule heating in all of the fuel cell components (including CL)

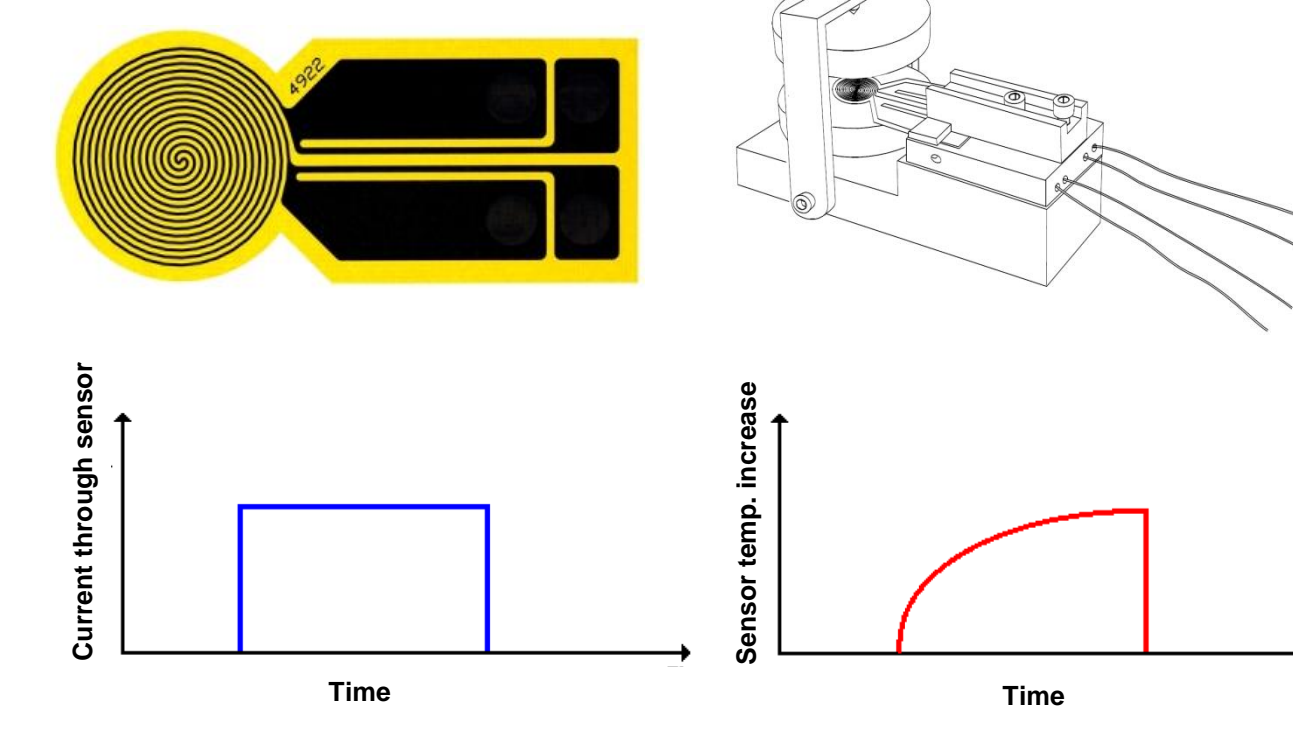
Local temperature variations affecting drying, flooding, and degradation phenomena

In situ temperature distribution are obtained from comprehensive mechanistic thermal conductivity models

Thermal Properties Measurements

Transient plane source (TPS) thermal analyzer

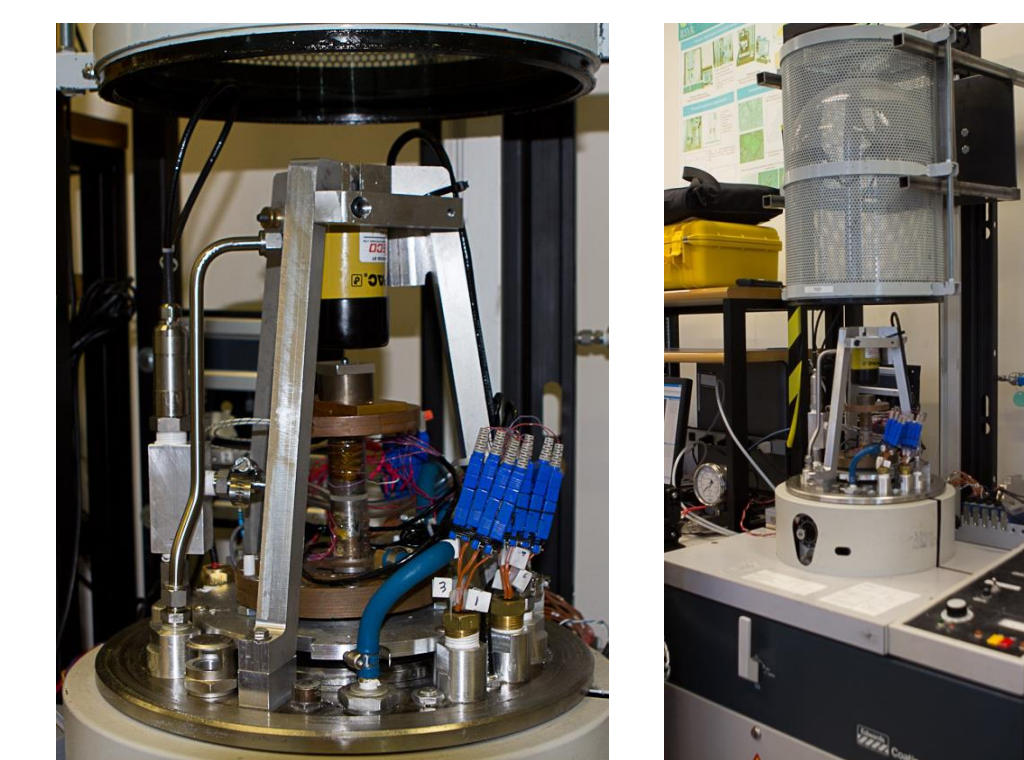
- Utilizes a thin foil double-spiral of nickel to resistively heat the sample and monitor the temperature change as a function of time
- Bulk materials, thin films, liquids, powders and pastes
- Isotropic and anisotropic materials
- Determines thermal conductivity, thermal diffusivity and specific heat
- Thermal conductivity range of 0.005-1800 W/(m·K)
- Accuracy: $\pm 5\%$
- Reproducibility: $\pm 2\%$
- Temperature controlled chamber (-35 °C to 200 °C)



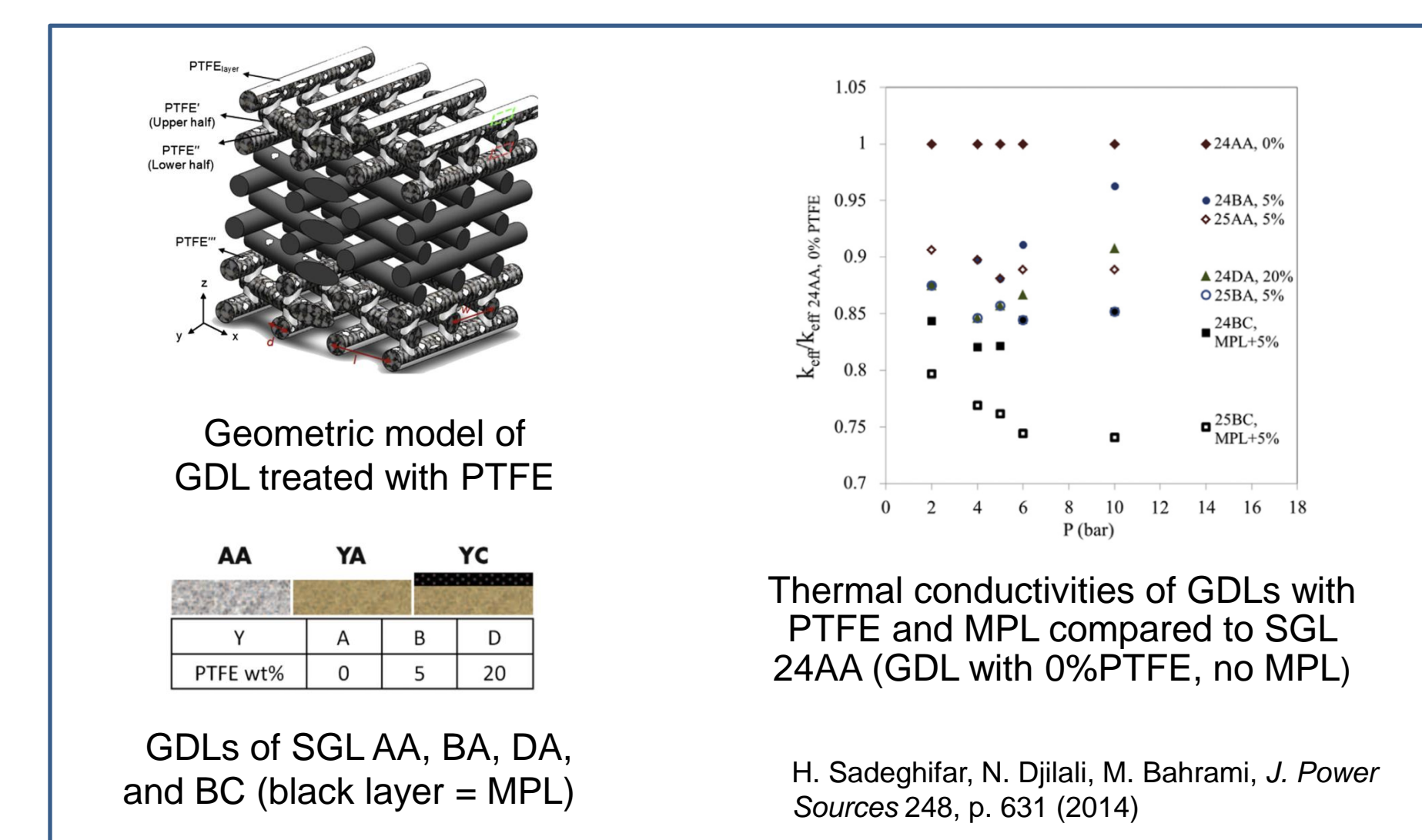
Transient Plane Source (TPS) 'Hot Disk' thermal conductivity, thermal diffusivity and specific heat analyzer

Guarded hot-plate thermal properties testing

- Steady-state measurement of heat flow through sample compressed between hot and cold plates
- Measurement of thermal conductivity and thermal contact resistance
- Thermal conductivity range of 0.1-10 W/(m·K)
- Hydraulic sample compression
- Laser interferometric displacement measurement
- Vacuum system to eliminate convection
- Sealed flow cell for sample testing with controlled relative humidity



Custom-built guarded hot-plate instrument with compression control to measure thermal conductivity and thermal contact resistance



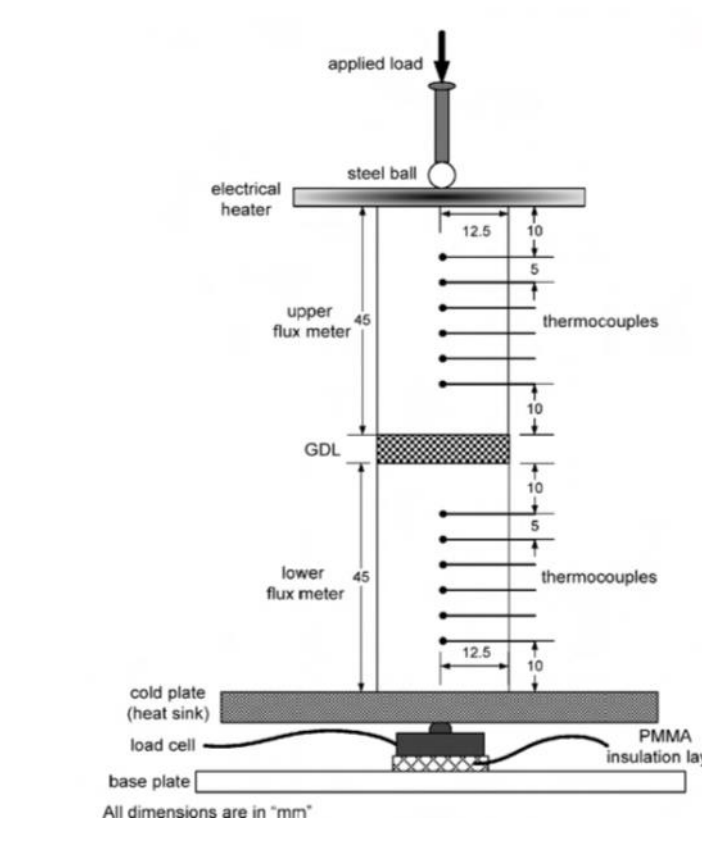
Geometric model of GDL treated with PTFE

AA	YA	YC
7	8	0
4	5	20
PTFE wt%	0	5

GDLs of SGL AA, BA, DA, and BC (black layer = MPL)

Thermal conductivities of GDLs with PTFE and MPL compared to SGL 24AA (GDL with 0%PTFE, no MPL)

H. Sadeghifar, N. Djalili, M. Bahrami, J. Power Sources 248, p. 631 (2014)

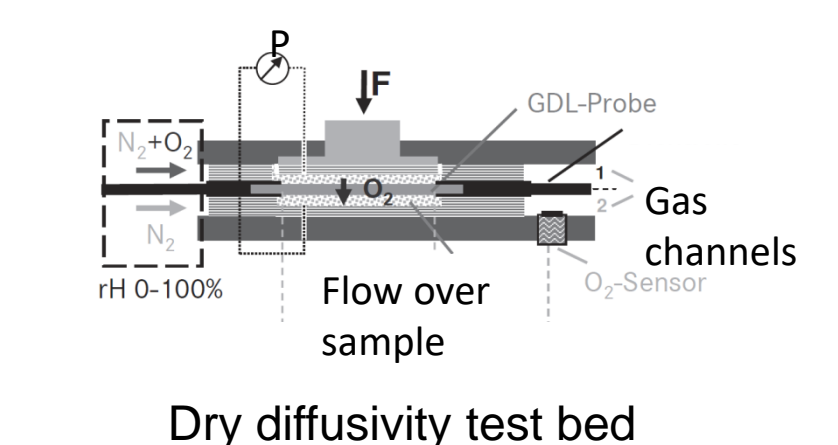


Schematic of guarded hot-plate thermal properties analyzer

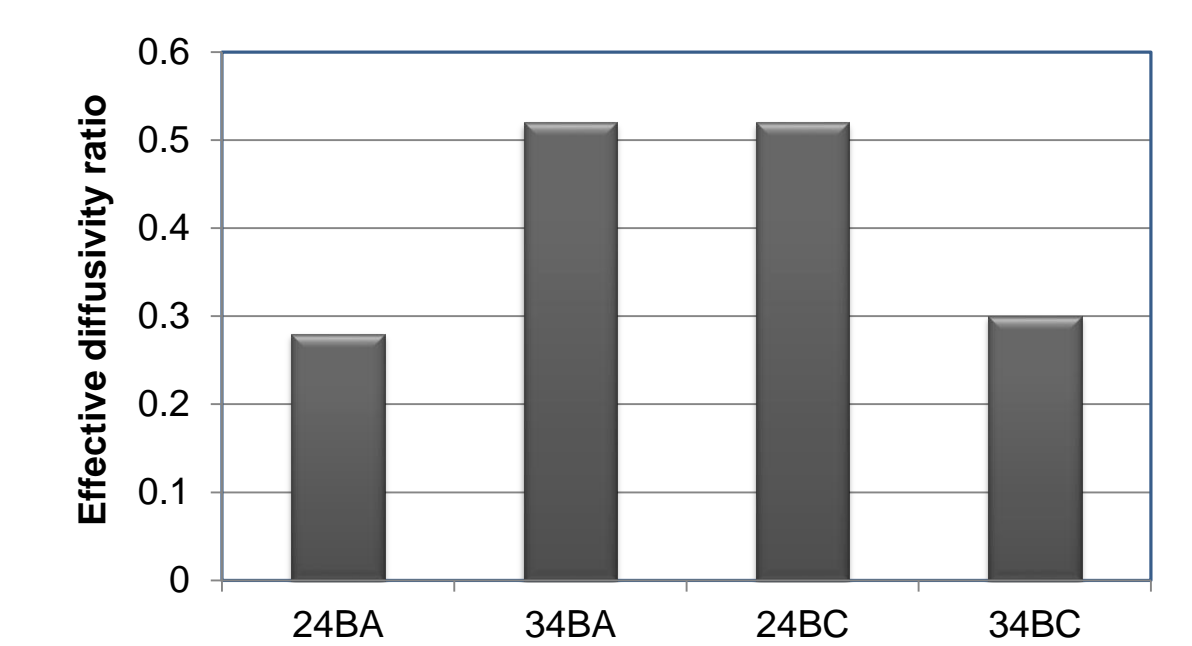
Diffusivity Measurements

Dry Diffusivity Test bed

- Two different known gas flows pass steadily over a thin porous sample
- Each gas penetrates through the sample
- The steady state concentration of each gas in the other flow is measured
- Based on a theoretical method the mass transfer resistance of the sample is calculated
- Knowing the thickness of the sample, the effective diffusivity is calculated

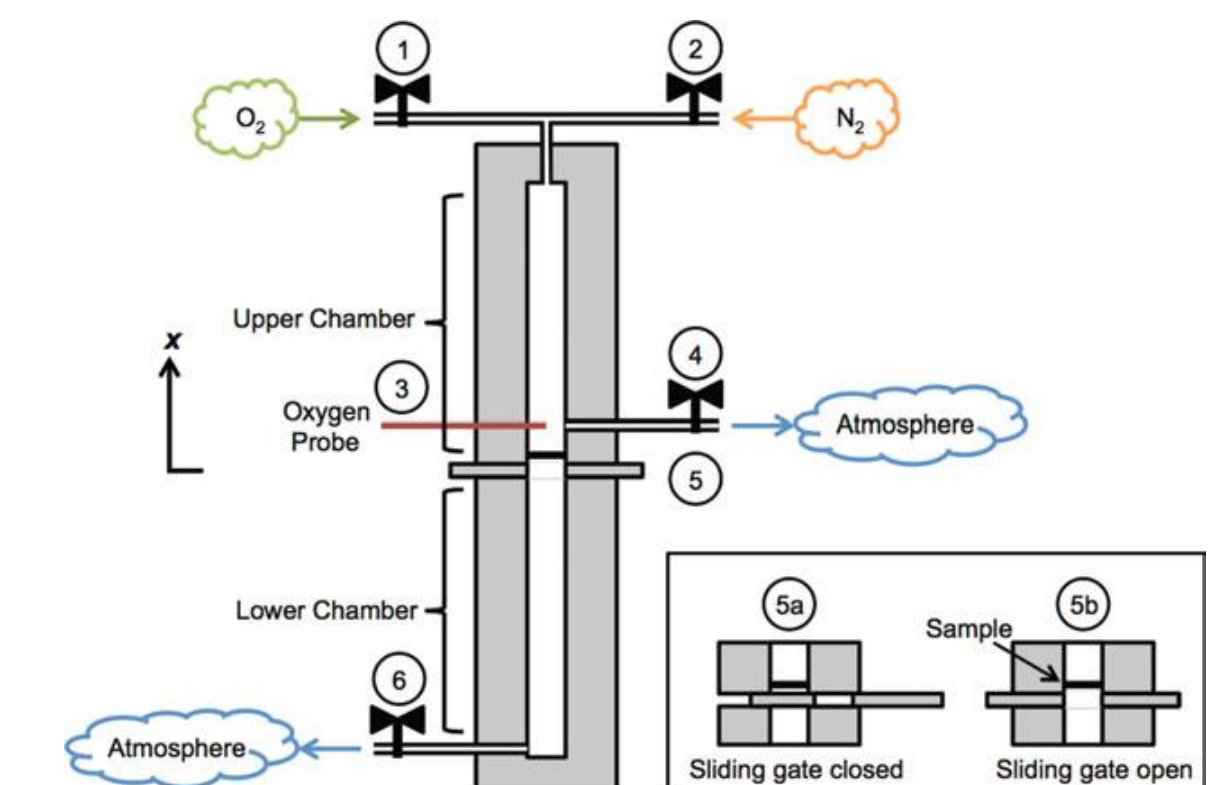
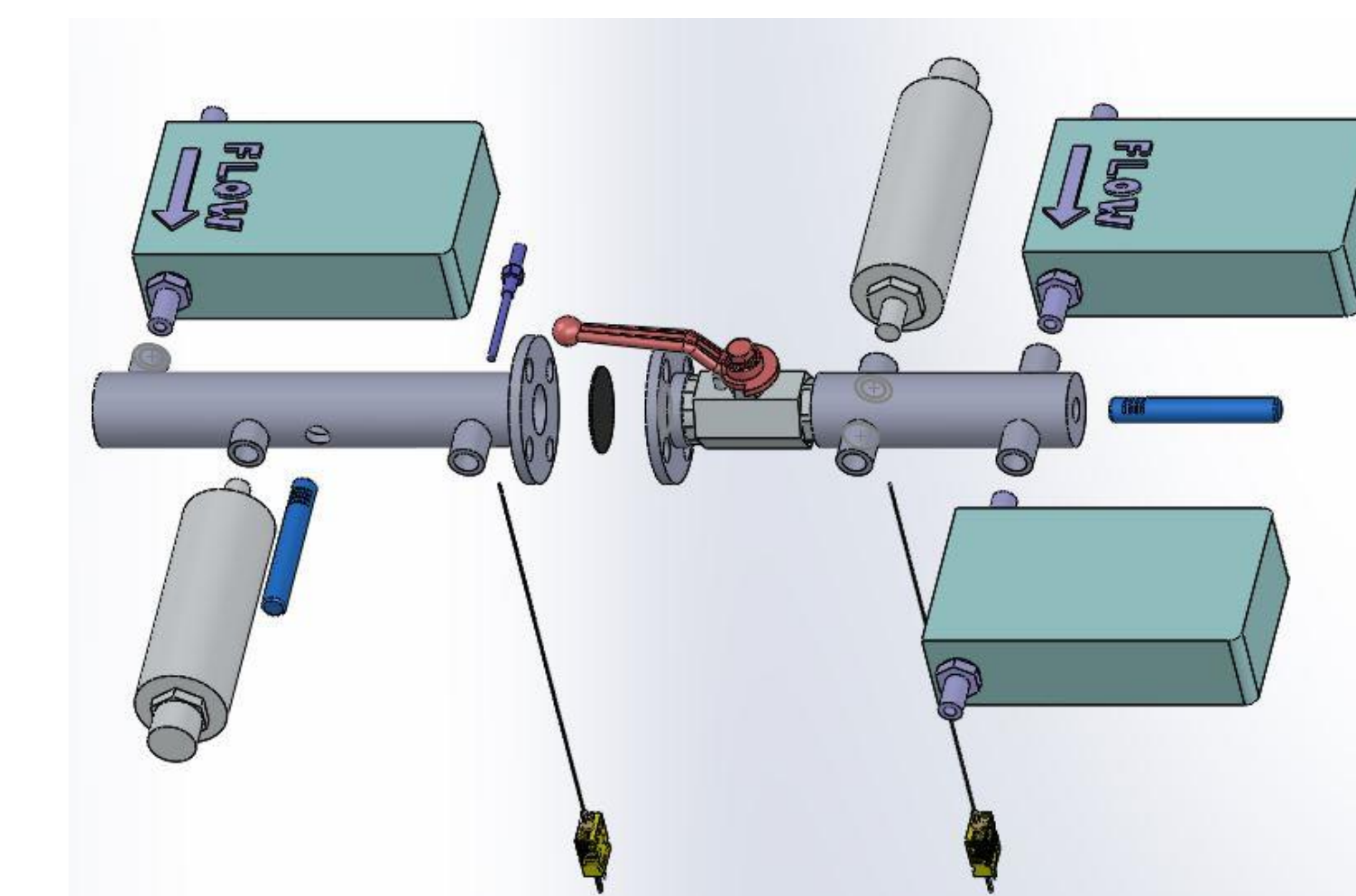


Dry diffusivity test bed



Modified Loschmidt Cell

- Two chambers filled with different gases
- A thin porous sample and a closed valve is between chambers at $t=0$.
- Valve is opened at $t=0$ and each gas starts to penetrate the other chamber through the sample
- Concentration of each gas at a specific location is measured as a function of time
- Based on a theoretical method, mass transfer resistance of the sample is calculated
- Knowing the thickness of the sample, the effective diffusivity is calculated



Schematic of the Loschmidt cell diffusion instrument

Support

