Simulation and Modeling for the Improvement on the Thermal Fluid Management of PEM Fuel Cell

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Research Goals and Objectives

The object:

Develop a computational model to predict the thermal/fluids transport on the anode side of the fuel cell with an emphasis on mass transfer enhancement.

Goals:

a) Develop a 3-dimensional simulation model using lattice Boltzmann equation (LBE) method that can be applied simultaneously to solve the flows in the channel and the porous media in the GDL.
b) Exploring alternative designs of the flow channel geometry using the model.

Relevance to Current State-of-the-Art

- Transversal flow across the GDL can be enhanced by placing flow enhancers in the channel. The resultant design is called *Inter-digitated Design*.
- There is a lack of systematic study that combines fluid dynamics in the channel and GDL and the electrochemistry on the surface of the membrane to characterize the modified flow.
- Modeling on the flow through porous media in the GDL is often based on empirical input such as permeability and ignores the roles of specific geometric details of the porous structure.
- LBE method can handle complex geometry (such as porous media and multiple flow blockers) with ease. It is powerful because it can automatically integrate the flow dynamics in the GDL with that in the channel.

Relevance to NASA

- The development of high power density and high energy density fuel cell systems is of significant interest to NASA space science missions as well as ground based mobility applications.

- Enhancing the mass transfer on the anode side of the fuel cell can help to achieve a significant enhancement of power density and energy density with commercially available PEM fuel cell systems.

Budget and Schedule

- Budget: $63,356
- Quarterly Tasks and Milestones for the first year

1. Develop 3-D LBE code for channel flow with partial flow blockers.
2. Develop 3-D LBE code to handle the 3-D GDL geometry.
3. Integrate the boundary condition on the membrane side for the electrochemistry.
4. Perform systematic simulations for flow going through the channel and GDL to assess the effect of the partial flow blockers and to optimize the design.
5. Develop a physical model for the transversal flow enhancement.

Deliverables

- A three-dimensional LBE code for simulating flow in the channel and in the GDL on the anode side will be developed.

- Based on the computational results, a physical model will be also developed to relate the enhancement of the transversal flow to the geometric parameters characterizing the flow enhancers, the permeability of the GDL, and the electrochemical conditions.

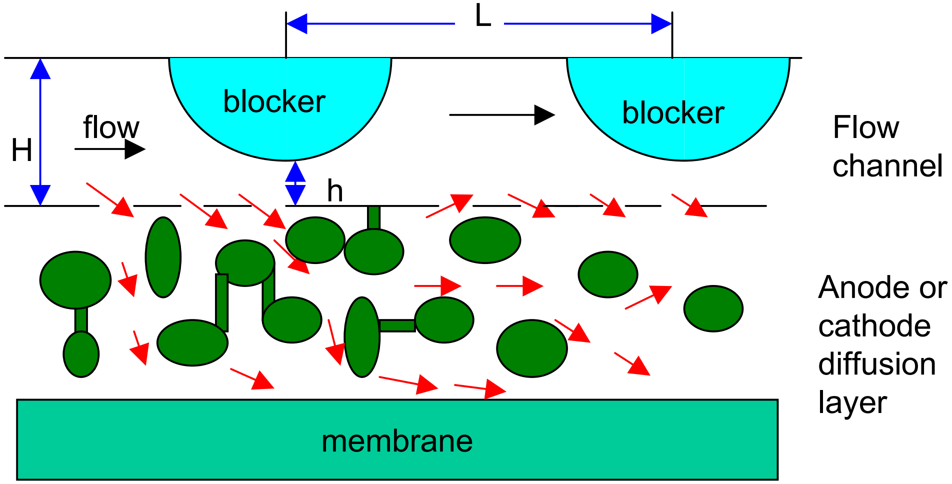
- Suitable design guidelines to enhance transversal flow in PEM fuel cell.

Anticipated Technology End Use

- Provide guidelines for the design of geometric parameters characterizing the flow channel, the flow enhancers, the permeability of GDL, and the electrochemical conditions in PEM fuel cell systems.

- The shear due to the enhanced transversal flow in GDL on the cathode side can help to remove water.

Approach to Enhance the Transversal Flow



An alternative arrangement of the flow blockers in the channel (not to scale)

- Fuel and oxygen in PEM fuel cell mainly flow in the direction that is parallel to the channel. The direction of the flow across the GDL is transversal.
- The desired transport of the fuel and oxygen is primarily associated with the transversal diffusion.
- By placing enhancers in the channel, the flow is forced to change direction (to the transversal direction), the transport of the fuel/oxygen across the GDL can be enhanced.

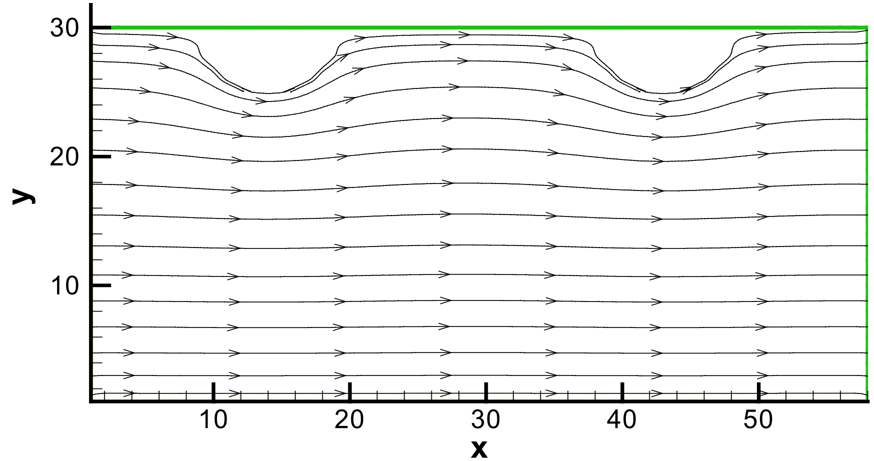
Accomplishments and Results

Completion of 3-D LBE code for channel flow with multiple flow enhancers

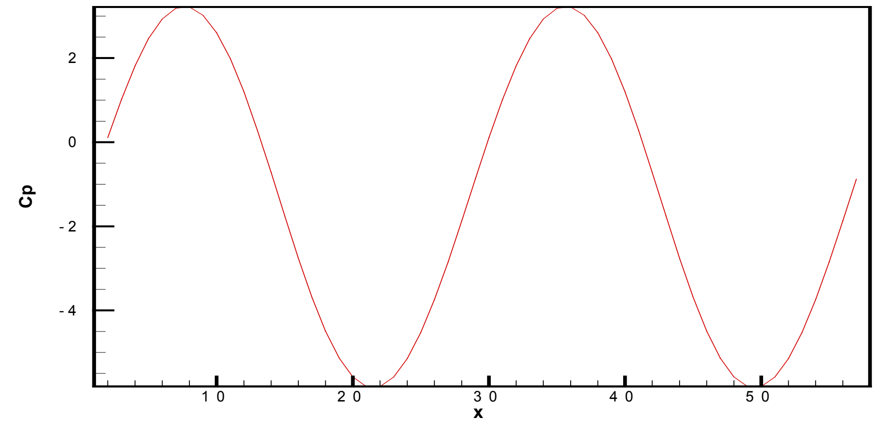
- The computational domain consists of the entire flow channel.
- Flow enhancers are placed in the flow channel.
- A 3-D LBE model (Q19D3) is used in the simulation.
- It solves the particle distribution function *fi (i=0,1,…,18)* in the flow domain.

Accomplishments and Results

- The flow is driven by a pressure gradient in the channel.
- Periodic boundary conditions for *fi* are imposed at the inlet and outlet of the channel. No-slip boundary conditions are imposed at all other four boundaries of the channel.
- Flow in the channel is forced to change direction and the pressure distribution on the lower boundary is not uniform.



Streamlines for flow channel



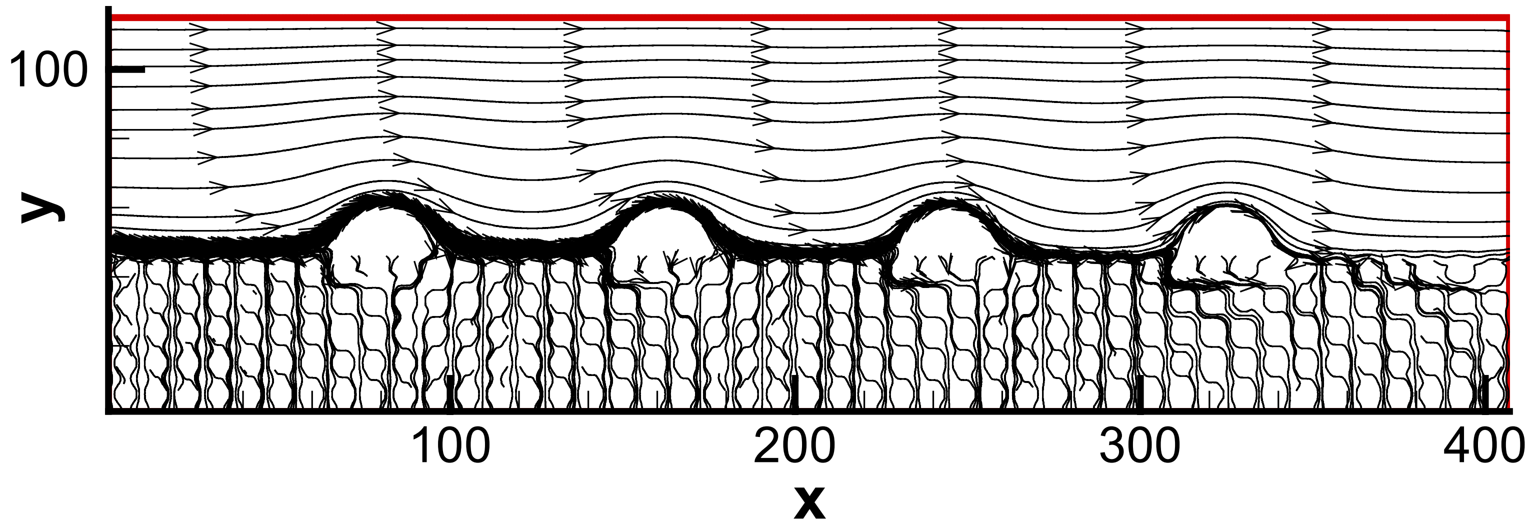
Pressure coefficient distribution on the lower boundary

Accomplishments and Results

Develop 3-D LBE code for flow channel and GDL

- The computational domain consists of the flow channel and GDL to investigate the transversal flow across the GDL.
- Arbitrary structure can be placed in GDL to simulate the porous substrate.
- The transversal flow rate through the lower boundary of GDL can be obtained and compared.

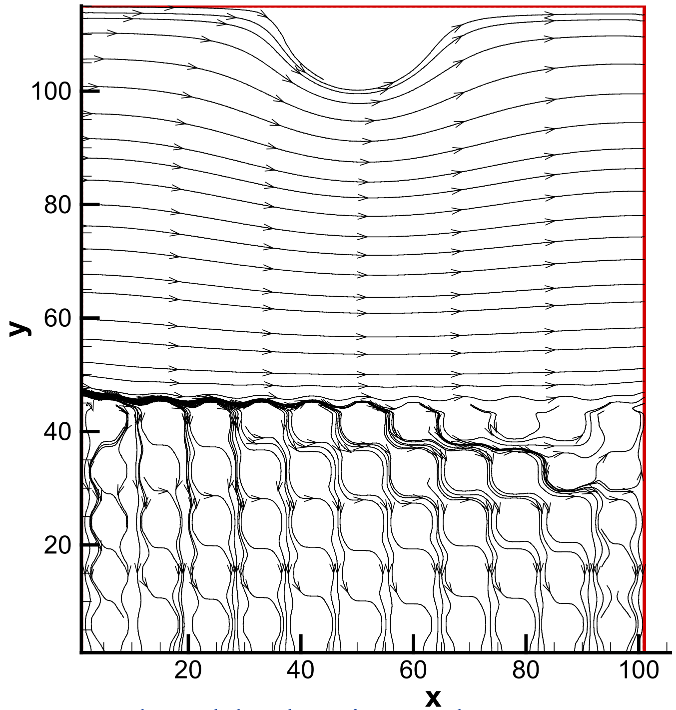
Accomplishments and Results



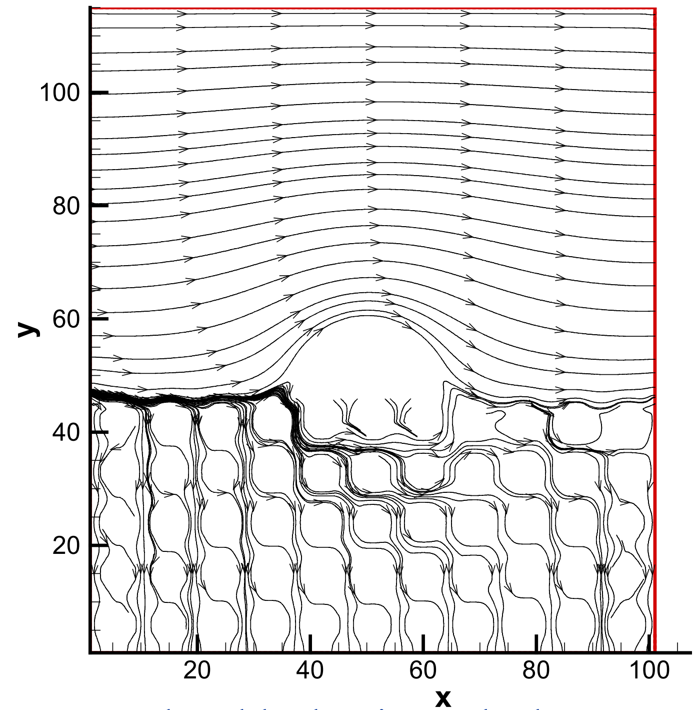
Streamlines for the flow in channel and GDL with multiple flow blockers

- Velocity at the inlet of the channel is given.
- Pressure at the outlet of the channel and on the lower boundary of GDL is specified.

Accomplishments and Results



Flow blocker is on the upper boundary of channel



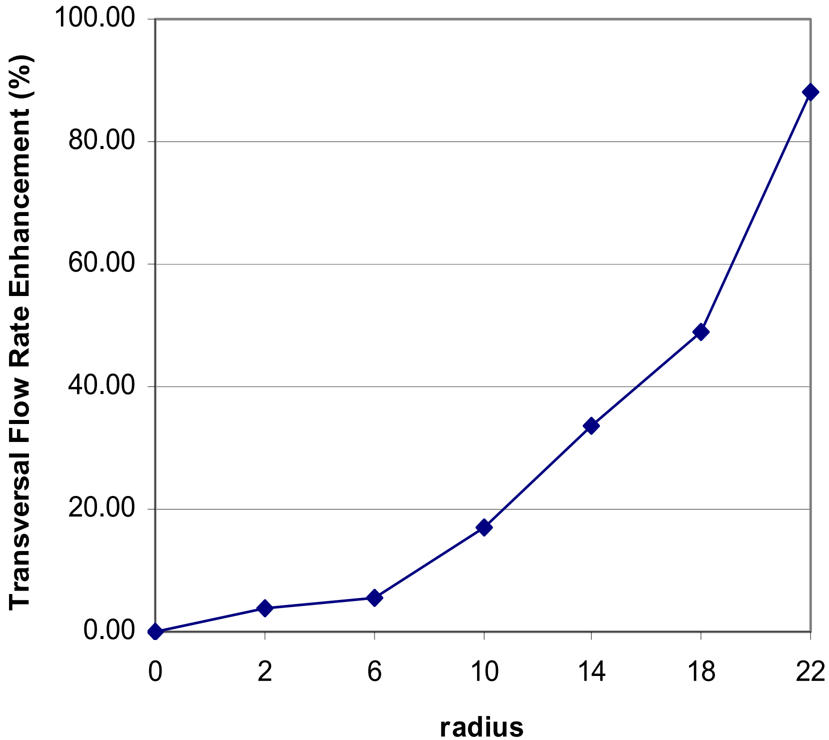
Flow blocker is on the lower boundary of channel

	enhancer on top	enhancer on bottom
Transversal flow rate enhancement	33.2%	33.6%

Transversal flow rate comparison

Accomplishments and Results

- The transversal flow across the GDL can be enhanced by placing flow enhancers in the channel.
- Increasing enhancer size => increase in transversal flow rate.
- Increase in transversal flow rate results from increased pressure drop through the channel.



Effects of enhancer size on transversal flow rate

Ongoing Work

Develop LBE code for mass diffusion in flow channel and GDL

- To integrate the boundary condition on the membrane side for the electrochemistry, the fuel gas diffusion needs to be considered together with the flow.
- The catalyst layer is simply regarded as a boundary condition. Integrate the boundary condition for the electrochemistry.
- Couple particle distribution functions *fi* (for fluid flow) and *gi* (for mass diffusion).

Ongoing Work

Boundary conditions for mass diffusion:

For the channel

$$\text{at } x = 0, \quad C = C_0$$

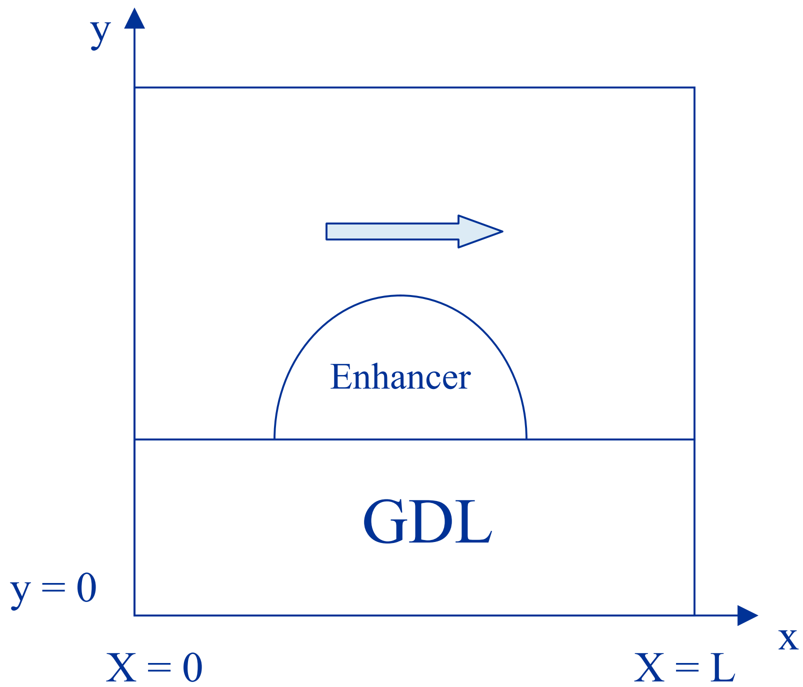
$$\text{at } x = L, \quad \frac{\partial C}{\partial x} = 0$$

For the GDL

$$\text{at } y = 0, \quad \frac{\partial C}{\partial y} = -\phi C$$

(Φ is the fuel cell electrostatic potential and based on electrochemistry)

On solid surface $\frac{\partial C}{\partial n} = 0$



Model of blocked flow channel

Future Plans

- Solve mass diffusion equation to integrate the boundary condition on the membrane side for the electrochemistry.
- Perform systematic simulations for flow going through the channel and GDL to assess the effect of the partial flow enhancers and to optimize the design.
- Develop a physical model for the transversal flow enhancement .