

Report of the 6th Meeting of the Transport Modeling Working Group

October 25 and 26, 2013

The Transport Modeling Working Group (TMWG) met over 1.5 days prior to the ECS meeting at Lawrence Berkeley National Laboratory (LBNL). The chosen topics were to discuss open source modeling and issues related to membranes and ionomers including thin films. The format was similar to previous meetings with ample time for discussion led off by a few presentations pertinent to the topic at hand. Both core TMWG participants as well as some experts and collaborators were invited to attend. The initial discussion focused on continuing to work on sections for the Critical Review article to be submitted to the Journal of the Electrochemical Society in the special modeling issue early in 2014.

Open Source

Several leaders in the fuel-cell open source modeling gave overview talks of their efforts including development of their own software. It was determined that even though there are different platforms being used, key is to have integration of the various codes. One aspect is that the codes themselves are not evolutionary and translatable among groups, something that open source and/or sharing could provide. However, such activities would require a community focus and also some dedicated effort to maintain and help with the codes at legacy type places (e.g., National Laboratories). It was stressed that for us to evolve as a modeling community, the key aspects for codes are:

- Modular and extendable codes
- Open source
- Freely available
- Usable from the user level with good documentation including test cases
- Standardize code development, documentation, etc.

There was also mention of a possible IEA Annex for modeling and open source modeling for fuel cells and hydrogen.

During the discussion, everyone seemed in favor of some kind of clearinghouse or sharing of codes such that we can stop reinventing the wheel each time a new person joins a group. This is especially true in situations where there are overlap of the physics and components between various codes. Some concerns and unanswered questions though regarding open source and sharing were brought up including:

- Are we supporting or competing against industry code people
- Are there issues because of licensing and export control
- Too many different codes so will not get consensus
- How to engage with industry such that they will use and build upon it both internally and in the community
- Do we need a completely common interface and platform

- Is the question and differences the modeling physics or is it modeling the various input properties
- How to engage in the larger (non fuel cell) but related communities (e.g., flow in porous media)
- The open source languages are not necessarily straightforward to adopt and use.

It was noted that open source is possibly a chance for DOE to lead this activity, especially for fuel cell R&D. One can also look at the work done by Jim Warren at NIST who is developing the infrastructure for the Material Genome and maybe leverage that effort which is supported by Department of Commerce. It was determined that we need a scoping document about the above ideas.

Action Item: Marc, Jon, and Adam work on scoping document for open source and modeling clearinghouse

Membrane Studies

In terms of modeling membranes, there were a couple of presentations concerning proton movement on ionomer-free services. Dr. Litster presented results of modeling that showed that charge is carried by both proton and hydroxide ions, especially within water within the double layer of NSTF pores. In order to do this requires including multistep kinetics and isotherms.

Dr. Borup then presented a question by the Fuel Cell Tech Team regarding the fact that membrane properties change over time and so there was some concern about how this impacts comparing experimental results among different membrane types. It is well known that PFSA's relax over very long timescales. The discussion then centered around whether this is an issue and if so, then how to resolve it. The concern is that waiting for relaxation may not make sense since we do not necessarily need the equilibrium values since those are not seen in practice. Some thought that then there should be two protocols including a rate dependent process (e.g., fast scan rates) and a pseudo-equilibrium one. The real question ends up being what are the timescales for property changes and that for relevant for operation. There is a need for more experimental data including perhaps some operation then tear apart and ex-situ testing to compare the membrane properties measured.

Action Item: Rod Borup to bring the discussion points back to the FCTT

Ionomer Thin Films

Dr. Weber, Karan, and Hickner discussed ionomer thin films both from recent experimental findings and from ways in which to model their effects. It was discussed that although we are now understanding thin-film morphology and uptake behavior with practical substrates, there is still a need to know what is happening at the various interfaces and bulk. Recent data show that thin films exhibit different confinement effects depending on their treatment, chemical structure, and thickness, where there is a decrease in uptake from bulk to 50 nm and then a slight increase around 20 nm and thinner. There is also a need to measure gas transport through the thin films as well. The article by Holdcroft in Chemistry of Materials was noted as a good source and discussion of these issues.

Next Steps

Final discussion centered around the TMWG, where again everyone agreed that it was a well-structured and useful meeting. Those attending it for the first time enjoyed the amount of discussion and the duration of 1.5 days that allowed for good interaction and collaboration. It was agreed that it should continue to be held alone and not as part of a conference where there are too many distractions. Similarly, a small group (~20) works out nicely for allowing good representation and discussions. Some of the keys for the success of the meeting and group included:

- Honesty about issues
- Keep it to a couple of issues
- Need to have industry participation
- Need to reach out to other communities and continue to have non-DOE-funded experts attend and talk.

A key outcome of the work has been the thin-film working group that has really taken the lead in the critical issue of properties of catalyst-layer thin films. For next meeting topics, some proposed were:

- Proton transport in NSTF and new CL architectures
- Time dependent properties and relaxation
- Ageing (which is perhaps related to the Durability Working Group)
- Dynamics/capacitance
- GDL/channel boundary condition
- Importance of interfaces?...multiscale
- Integration of models
- Multistep interactions and ORR and alloys, etc. (which should be with the Catalyst Working Group)
- Molecular scale issues including MD, DFT, etc. (should be related to BES activities).