OpenFCST: Fuel Cell Simulation Toolbox

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Fuel cell operation involves a myriad of coupled physical processes:
- Multi-component reactant gas transport
- Charge transport: Proton and electron transport
- Liquid water transport: Two-phase flow
- Heat transport
- Electrochemical reaction

Fuel cell mathematical models must account for all these physical processes simultaneously:
- Complex coupled problem
- "Constantly evolving" models
Introduction

➤ There is a need to develop a collaborative fuel cell mathematical modeling software that can be shared and “evolved” within the fuel cell community

➤ The mathematical modeling software should be:
  ❑ Multi-dimensional
  ❑ Modular and easy to extend
    ❉ New materials
    ❉ New physics
  ❑ Accessible to both users and mathematical model developers
What is OpenFCST?

- The Fuel Cell Simulation Toolbox (FCST) is an open-source mathematical modeling software for polymer electrolyte fuel cells.

- It is a toolbox that contains:
  - **Pre-processors:** A fuel cell specific grid generator and a class to read meshes from an open-source mesh generator (we use SALOME, i.e. UNV).
  - **Solvers:** Multi-dimensional FEM solvers and nonlinear solvers as well as libraries of materials, layers and physical equations. FEM routines provided by the deal.II open-source libraries.
  - **Post-processors:** Functional evaluation algorithms and a VTK file generator (we use ParaView for post-processing).
  - **Design and optimization capabilities:** Parametric studies, parameter estimation and optimization algorithms. Optimization functionality provide by Dakota.
Main components of the code

- Pre-processor

- Solver:
  - Application framework
  - Equation framework
  - Layer framework
  - Materials database
  - Reaction database

- Post-processor
Application framework

- Two main applications
  - Linear finite element applications
    - Generate and store mesh
    - Read parameter file and initialize equation, layer and material objects
    - Loop over cells and assemble the FEM global matrix and right hand side
    - Solve the linear system
    - Applications developed: cathode, MEA and Laplace models
  - Wrapper applications
    - Implements iterative solution strategies for adaptive refinement, non-linear solvers and transient algorithms
FEM application interface

1. initialize

FEM

2. assemble

3. solve

\[
\begin{align*}
\nabla \cdot (cD_{O_2}^{\text{eff}} \nabla x_{O_2}) &= S_{O_2} \\
\nabla \cdot (cD_w^{\text{eff}} \nabla x_w) &= S_w + S_{\lambda} \\
\nabla \cdot (\sigma_m^{\text{eff}} \nabla \phi_m) &= S_{H^+} \\
\nabla \left( n_d \frac{\sigma_m^{\text{eff}}}{F} \nabla \phi_m + \frac{\rho_{d_{w}}}{E W} D_{\lambda}^{\text{eff}} \nabla \lambda \right) &= -S_{\lambda}
\end{align*}
\]

\[
\begin{bmatrix}
  k_{11} & \cdots & k_{1N} \\
  \cdots & \cdots & \cdots \\
  k_{N1} & \cdots & k_{NN}
\end{bmatrix}
\begin{bmatrix}
  u_1 \\
  \vdots \\
  u_N
\end{bmatrix}
= \begin{bmatrix}
  f_1 \\
  \vdots \\
  f_N
\end{bmatrix}
\]
Equation framework

- Equation classes implement the weak form of the PDE that needs to be solved
- Currently implemented equations
  - Fick’s law
  - Ohm’s law
    - Electronic transport
    - Protonic transport
  - Water transport model
  - Reaction source term model
  - Thermal transport model (to be released this fall, openFCST 0.2)
  - Navier-Stokes equation model (not yet released)
  - Two-phase flow model – single equation (not yet released)
Layer framework

- Layer classes developed to compute:
  - Effective transport properties
  - Derivatives of effective transport properties
  - Multi-scale integration requirements
- Materials objects inside layer to estimate the effective properties
- If the layer is reactive, kinetics object stored and used to compute reaction rates
- Layer interface allows users to swap layers via the input file
Material database

- Material database contains information on:
  - Gases: $T_c$, $p_c$, enthalpy, entropy, etc.
  - Catalysts: Activation energy, transfer coeff., etc.
  - Catalyst supports
  - Fibers (for GDLs)
  - Electrolytes

- Materials of the same family can be swapped at real time
Fuel cell electrochemical reactions are complex, multi-step reactions involving many intermediates

- To date, a detailed mathematical model does not exist

An interface to explore novel kinetics has been developed

Currently it contains:
- A Tafel equation (simplest electrochemical reaction model)
- A Butler-Volmer equation
- A Double-trap multi-step kinetic model for the ORR
- A Dual-path multi-step kinetic model for the HOR
Mathematical fuel cell model

- Steady-state and isothermal
- Solving for:
  - Oxygen mole fraction
  - Electrolyte potential
  - Solid potential
- Governing equation:

\[
\nabla \cdot \left( c_{\text{tot}} D_{O_2}^{\text{eff}} \nabla x_{O_2} \right) - \frac{1}{4F} \nabla \cdot \vec{J} = 0
\]

\[
\nabla \cdot (\sigma_{m}^{\text{eff}} \nabla \phi_m) - \nabla \cdot \vec{J} = 0
\]

\[
\nabla \cdot (\sigma_{S}^{\text{eff}} \nabla \phi_S) + \nabla \cdot \vec{J} = 0
\]
Mathematical model: Electrochemical reactions

- Tafel model usually used in fuel cells
  \[ \nabla \cdot \vec{\mathbf{i}} = A_v l_0^{ref} \left( \frac{C_{O_2, g|l}}{c_{ref}^{O_2}} \right) \gamma \exp \left( -\frac{\alpha_c F}{RT} (\phi_s - \phi_m) \right) \]

- ORR is a multi-step reaction

Dissociative adsorption (DA): \( 1/2 O_2 \Leftrightarrow O_{ad} \)
Reductive adsorption (RA): \( 1/2 O_2 + H^+ + e^- \Leftrightarrow OH_{ad} \)
Reductive transition (RT): \( O_{ad} + H^+ + e^- \Leftrightarrow OH_{ad} \)
Reductive desorption (RD): \( OH_{ad} + H^+ + e^- \Leftrightarrow H_2 O \)

- The source term in the cathode is
  \[ \nabla \cdot \mathbf{i} = j_k = j^* e \frac{-\Delta G_{RD}^*}{kT} \theta_{OH} - j^* e \frac{-\Delta G_{-RD}^*}{kT} (1 - \theta_O - \theta_{OH}) \]
  \[ \Delta G_{RD}^* = \Delta G_{RD}^0 + \beta e \eta \quad \Delta G_{-RD}^* = \Delta G_{RD}^0 + \Delta G_{OH}^0 - \beta e \eta \]

  where \( \eta = \phi_s - \phi_m - E_{eq} \)

Mathematical model: Electrochemical reactions

- Tafel plot shows the effect of the kinetic model
  - Doubling due to kinetics
  - Doubling due to mass

- Effect of kinetic model clearly visible in reaction rate distribution @1A/cm²
  - Layer is less reactive, i.e. higher utilization
Mathematical model: Electrochemical reactions
MEA model and experiments (80°C, 70%RH)

- Scale-up cathode model to full MEA simulation with micro-scale model
- MEA model based on Tafel over predicts performance for thin electrodes
- Double-trap model is able to predict voltage losses accurately
Effect of varied micro-structures in cathode electrode

Effect of varied micro-structures in cathode electrode

- Agglomerate parameters:
  - $R_{agg} = 100$ nm
  - $\delta_{agg} = 5.62$ nm
  - 20% porosity

- Macro-homogeneous and agglomerate models show similar performance

- Water-filled model only appropriate if catalyst is negatively charged
Effect of varied micro-structures in cathode electrode

- Graded Platinum distribution:

- Ionomer interfacial resistance:

- Polydispersion of agglomerates:

Patterned Electrode Analysis

- Inkjet printing used to pattern electrodes
- Effect of thickness and spacing between printed CL blocks analyzed in openFCST
- Reaction hot-spots observed
Conclusions

➢ An open-source numerical analysis framework has been developed for analyzing multi-dimensional fuel cells
  ❑ Modular and easily extendable
  ❑ Developed for (users and) developers
    ○ Release 0.2 (due November) will contain a GUI and will use CMake to improve installation issues in different environments
  ❑ Developed in C++ using a Linux environment
  ❑ Caution: Steep learning curve (but we are willing to help)

➢ The framework has been successfully applied to analyze:
  ❑ Different electrochemical reaction models
  ❑ Different micro-scale models
  ❑ Perform three-dimensional catalyst layer simulations of patterned electrodes
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Catalyst layer and membrane electrode assembly models

FCST contains several ready-to-use fuel cell models as well as toolboxes for electrical, ionic, and gas transport models.