RF regressors (RFR): non-linearities provide straightforward methods for feature selection. Random forests (RF) are popular ML methods due to their proven accuracy, stability, and ease of use, and are used to study long-term or inter-term operating effects. Speeding up stack performance simulations by coupling multi-physics problem to obtain a reduced number of inputs while maintaining physical interpretation: physics-based machine learnt model.

Critical challenges are their long-term durability and material degradation processes, and thermal management. Feature engineering analysis of Multiphysics problem to obtain a reduced number of inputs while maintaining physical interpretation: physics-based machine learnt model.

Train the RFR with all features for an increasing number of trees (N)$^*$ and compare Out-of-Bag (OOB), train and test error rates. No. features$^*$=18

Table 2. Comparing PDE vs ML model for different temperatures and same feed compositions.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$_2$ reaction order</td>
<td>0.28</td>
</tr>
<tr>
<td>H$_2$ reaction order</td>
<td>0.28</td>
</tr>
<tr>
<td>O$_2$ reaction order</td>
<td>0.198</td>
</tr>
<tr>
<td>E$^\circ$ (V)</td>
<td>44.686.47</td>
</tr>
<tr>
<td>E$^\circ$ (V)</td>
<td>94.325.81</td>
</tr>
</tbody>
</table>

Validation against Multiphysics model and Literature data

PDE vs ML: Reversible solid oxide cell (SOC)

Reasonably good agreement for operation at higher temperatures. As temperature decreases and current density increases deviation from PDE overpotential solution is observed. ML model captures the effect of feed composition changes for "well" trained cases. Initial validation with literature data shows cell potential mismatch at high temperature. Possibly, lack of enough polarisation data points for specific combination of physical parameters/features.

Next steps

- Expand data generated to capture the effect of individual physical parameters and their combined effect.
- Evaluation of other ML alternatives or their coupling with the RFR for better guess in regions with reduced polarisation points.
- Validation against extensive experimental data: ESC, ASC, MSC.
- Test methodology on other systems like PCFC.
- Coupling with hierarchical multiscale modeling framework to allow for lifetime simulation.

References