Mechanistic Mathematical Model for Deactivation of Catalysts in Direct Internal Reformer in Molten Carbonate Fuel Cells

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Molten carbonate fuel cell (MCFC) technology has been commercialized by FuelCell Energy, Inc. using the DFC® (Direct Fuel Cell) technology. Unlike alkaline, phosphoric acid, and polymer electrolyte membrane fuel cells, DFC® uses internal steam reforming of methane to produce hydrogen within the fuel cell module, shown in figure 1. This configuration thus has the advantage of high thermal efficiency by thermo-chemical integration of direct internal reforming (DIR) and indirect internal reforming with the electrochemical anodic reaction.

A key challenge in MCFC is the accelerated deactivation of the DIR catalyst in the presence of the molten carbonate electrolyte at the normal operating temperature of about 650 °C. This accelerated deactivation of the DIR catalyst will limit the fuel cell life. The activity of the catalyst is significantly reduced (>70%) in the carbonate electrolyte environment. During operation electrolyte is transported to the catalyst by creep from the electrode or by deposition of electrolyte vapor. The deactivation in the presence of electrolyte is widely believed to be caused by electrolyte aided sintering, coverage of catalyst surface, blockage of pores, and metal oxides solution formation [1-6].
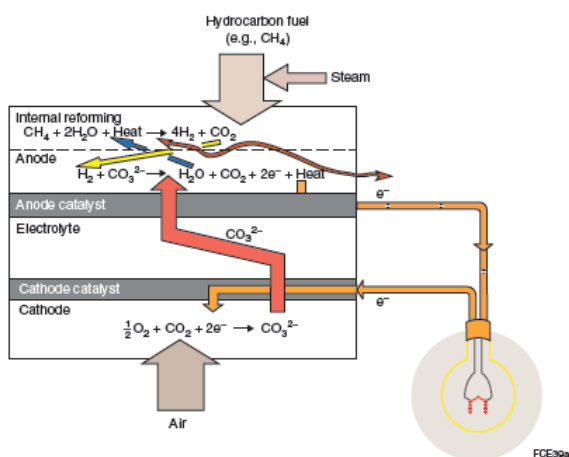

Fig. 1 Conceptual configuration of internal reforming unit in DFC®.

Understanding the contributions of each of the above factor that affect catalyst deactivation becomes important to identify best approaches to improve the stability of the DIR catalyst.

This work discusses the development of a mechanistic model for deactivation of DIR catalyst in MCFC to understand and quantify the effects of different poisoning mechanisms, like loss of area by sintering, coverage catalyst surface by electrolyte and blockage of pores.

Activity of a catalyst pellet is modeled by considering the physical properties (porosity, surface area) of the pellet. The total activity loss is directly correlated with active surface area within the catalyst, and takes into account losses from sintering, surface coverage /or pore plugging of DIR.

While sintering does reduce the surface area of the catalyst, electrolyte coverage and pore blockage are important factors that cause large reduction in activity of the catalyst. If electrolyte transport to the catalyst is reduced or if the catalyst is made resistant to the electrolyte, loss of activity can be substantially reduced.

Electrolyte pickup of the catalyst is a critical measurement of the transport to the catalyst or the resistance of the catalyst. A series of electrolyte pickup tests were performed to characterize pickup in the conventional catalyst. A few different modifications were done to the catalyst to change the resistance to electrolyte. A few of the modified catalysts showed significant reduction in the electrolyte pick up, shown in fig. 2.

Electrolyte pick up test is used as a screening tool. Further stability investigations are planned in the future.
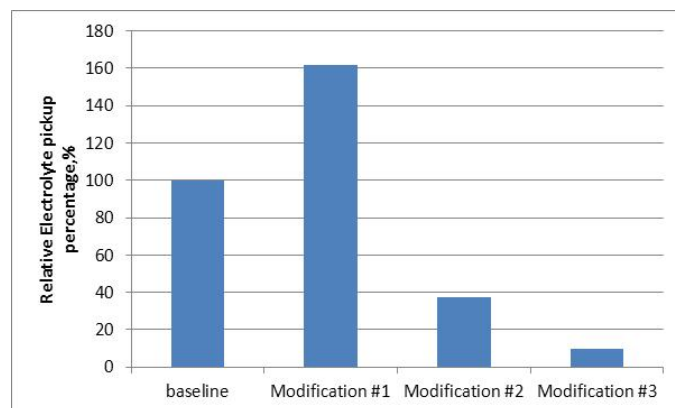

Fig. 2 Effects of modifications on the electrolyte pickup rate for DIR catalyst in MCFC.

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