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Design and Simulation for Fuel Cell Cathode Air Filter

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Abstract

Proton exchange membrane (PEM) fuel cells experience performance degradation, such as reduction in efficiency and life, as a result of poisoning of platinum catalysts by airborne contaminants. The best method for addressing fuel cell air contamination is by the inclusion of adsorptive filtration with a cathode air filter. In this paper, simulation for chemical adsorption behavior of air filter has been studied, which is based on Fluent. The adsorption of SO₂ was simulated in the air filter, which structure was designed and optimized for a 5kW fuel cell stack system. Not only the distribution of SO₂ capacity with time in filter could be shown, but also the durability of filter can be evaluated. Furthermore, the velocity of flow and pressure drop of filter also were simulated. The simulation study for chemical adsorption and hydrodynamics in fuel cell cathode air filter help to optimize air filter to be durable and effective.

Keywords:Simulation, Chemical Adsorptive, Air Filter, PEM Fuel Cell

1. Introduction

Proton exchange membrane fuel cells (PEMFCs) are being developed as an alternative to the internal combustion engine (ICE) for automotive propulsion in order to reduce fossil fuel consumption. However, air in these operating environments may contain contaminants that are damaging to fuel cell performance, especially once emitted from ICE vehicles [1]. There have been many studies regarding the impact of various air contaminants[1–5]. For example, 1 ppm of NO₂ could reduce fuel cell performance by 10% while the same concentration of SO₂ caused a 35% loss of cell voltage within 100 h [2]. Hundred and forty parts per million of NO_x (NO:NO₂ = 9:1) could cause a 30% reduction in cell voltage within 5 min [1]. However, the effects of CO and hydrocarbon (i.e. benzene and propane) were less severe than those of NO_x and SO₂ [4,5]. Furthermore, the performance of fuel cells could not be fully recovered after poisoning by NO_x or SO₂. Therefore, it is a challenge to prevent the cathode from the contamination of NO_x and SO₂ in air when operating fuel cell vehicles in real environment.

Two methods for dealing with contaminated air effects on fuel cell cathodes are to increase catalyst durability and/or to filter contaminants from the air. Because of the wide variety of contaminants, increasing membrane resilience by modifying the catalyst or increasing the catalyst amount is a difficult and possibly expensive alternative. Therefore, the most effective and flexible method for operating fuel cells in contaminated environments is adsorptive filtration of contaminants from the ambient air stream[5].

The designing parameters of an adsorptive filter, including saturation capacity, removal efficiency and pressure drop, depend on the inlet air properties (contaminants, concentration and air flow rate), filter design options (packed bed or micro-fibrous material) and filter footprint (area, thickness and weight) [6].

In the present work, simulation for chemical adsorption behavior of air filter has been studied, which is based on Fluent. We simulated the adsorption of SO₂ in the air filter. Not only the distribution of SO₂ capacity with time in filter could be shown, but also the durability of filter can be evaluated. Furthermore, the velocity of flow and pressure drop of filter also be simulated. The simulation study for chemical adsorption and hydrodynamics in fuel cell cathode air

filter help to optimize air filter to be durable and effective.

2. Methodes

In this paper, granular activated carbon (GAC), modified by KOH, has been used as adsorptive material to filtrate the air contaminations. AC was first put in a furnace under helium atmosphere at 800 °C for 1 h to remove possibly contained volatiles, and then impregnated into KOH solutions at 0.5M/L KOH concentration with stirring for 3 h at 45 °C, followed by dehydration in a vacuum oven at 100°C for 8 h. Finally, ten adsorbent samples including the original AC sample were prepared and kept in a desiccator.

The prepared adsorbent was filled in the bed reactor and the adsorption behavior has been tested in the home-made test-bench. The Schematic diagram of experimental set-up was showed in Figure 1.

Figure 1. Schematic diagram of experimental set-up

According to the 3D mathematic model, CFD software Fluent has been applied in the air filter structure optimized design. The porous medium model and chemical adsorptive model based on UDF was set and chemical property of air filter element has been calculated in this paper.

3. Results and Discussion

3.1 Effects of inlet Properties on adsorption

The air flow rate of fuel cell vehicle depends on the system power; while the initial concentration of contaminations relies on atmosphere quality. These parameters are pivotal on the filter. So the effects of inlet properties on filter adsorption have been tested, the results have showed in Table.1. The results indicated that the breakthrough time decreased with the increase of initial concentration in the same airflow rate, and the breakthrough time also decreased with the increase of air flow rate in the same initial concentration.

Table 1 Effects of inlet Properties on adsorption

Initial Concentration (ppm)	Air flow rate (m/s)	Breakthrough time (min)
13.2	0.088	380
20.1		248

38.8	0.175	152
62.0		78
6.0		244
13.1		148
22.5		98
34.5		70
48.8		49
6.2	0.350	140
22.0		47
31.5		37
40.0		25
2.3	0.701	104
4.2		50
8.0		23
20.0		15
40.5		14

3.2 Mathematic Model

The adsorption mathematic model was founded based on the experimental data. The Wheeler formula (1) has been introduced to found the adsorption model.

Wheeler formula is showed as flow:

$$t_b = \frac{q\rho_b}{C_0Q} \left(H - \frac{Q}{k_v} \ln\left(\frac{C_0}{C_x}\right) \right) \quad (1)$$

t_b is breakthrough time, q is equivalent adsorption weight, ρ_b is density of GAC C_0 is initial concentration, Q is air flow rate, H is bed ply, k_v is adsorption speed constant, C_x outlet concentration for breakthrough. Figure 2 showed the Wheeler Equation fits according to the experimental data.

Figure 2 effects of breakthrough time on initial concentration at different flow rate

The Datafit software was used in the paper and the 3D mathematic model has been founded, which was showed in figure 3. The breakthrough time can be calculated on the certain inlet concentration and flow rate according to this 3D model, which is in the area of initial concentration and airflow rate.

Figure 3 3D model for breakthrough time-inlet concentration-flow rate

Figure 4 showed the simulated result and experiment data and the hollow symbol is simulated result and the other is experiment data, which showed the simulation accorded with the experiments.

Figure 4 Comparison between simulation and experiment data for GAC adsorption.

3.2 Simulation for Air Filter

According to the 3D mathematic model, CFD software Fluent has been applied in the air filter structure optimized design for a 5kW fuel cell stack system. The porous medium model and chemical adsorptive model based on UDF was set and the hydrodynamic and chemical property of air filter has been calculated in this paper. Figure 5 showed the distribution of velocity of flow in filter, the result showed that the distribution of velocity is uniformity, the range is about 0.14m/s-0.29m/s well-proportioned distributed in the filter and only the maximal air velocity in the air filter reached about 14m/s in export. Figure 6 showed the distribution of pressure drop in filter. About 3719Pa of the pressure loss was obtained, which is in the acceptable range for pressure drop in filter.

Figure.5 Distribution of velocity of flow in air filter

Figure.6 Distribution of pressure drop in air filter

Figure 7 showed the distribution of SO₂ capacity with time in air filter. The SO₂ adsorption in filter reached the saturation with time. Furthermore, the saturation capacity of SO₂ is distributed uniformly in the filter, which attributed to particular design for the air filter. The life time of filter is about 1203 hours, which can protect the fuel cell well. So the simulation study for chemical adsorption and hydrodynamics in fuel cell cathode air filter help to optimize air filter to be durable and effective.

(a) 20 hours

(b) 400 hours

(c) 1100 hours

(d) 1200 hours

Figure 7 Distribution of SO₂ capacity with time in air filter

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Graduated from Shanghai Jiaotong University and obtained a PH.D degree. Now, the research field focuses on hydrogen and fuel cell technology.

4. Conclusion

The design and simulation for fuel cell cathode air filter has been studied in this paper. A three-dimension mathematic model between inlet property and adsorption property was built based on the GAC adsorptive experiment data. The breakthrough time can be calculated continuously and correspondingly in the area of initial concentration and airflow rate. According to the 3D mathematic model, CFD software Fluent has been applied in the air filter structure optimized design for a 5kW fuel cell stack system. About 3719Pa of the pressure loss was obtained and the life time of filter element is about 1203 hours. This air filter realized the design goal and can protect the fuel cell well.

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