Numerical simulation of internal flow and adsorption process in an activated carbon canister for ORVR system

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Abstract. In the vehicle fuel evaporation control system, the activated carbon canister is the core component and plays a vital role in the performance of the entire system. In this paper, a numerical simulation of the internal flow and adsorption process of an activated carbon canister used in an ORVR system was conducted to analyze the influence of the structure of the canister on the flow distribution and adsorption process. The research results showed that in the adsorption process, the flow through the activated carbon layer belonged to laminar flow, which was conducive to the full absorption of butane by activated carbon. In the desorption process, the flow velocity reached 0.05-0.09m/s. The higher flow velocity was beneficial to the desorption of the activated carbon. In the initial adsorption stage, due to the high flow velocity through the inlet, the butane concentration distribution was non-uniform, and the activated carbon under the inlet saturated faster than other positions. The activated carbon released heat during the adsorption process. The temperature at each monitor point showed a trend of fast increasing first and then slowly decreasing. The adsorption capacity of each monitor point increased significantly in the early stage of the adsorption process, while in the later stage tended to be stable. The adsorption capacity of butane was directly affected by the temperature of the activated carbon layer. The higher temperature was not conducive to the adsorption process.

1. Introduction
With the implementation of the Limits and Measurement Methods for Emissions from Light-duty Vehicles (China 6) in 2016, the requirements for energy saving and emission reduction of automobiles have become more stringent. The vehicle fuel evaporative emissions control is one of the important contents of the emission regulation of China 6. The vehicle fuel evaporative emissions mainly refer to the fuel vapor emitted from the fuel supply system composed of the fuel tank, fuel filter and fuel pipelines, which mainly include running losses, diurnal losses, hot soak losses and refueling losses [1]. At present, the main method of controlling vehicle fuel evaporative pollutants is the vehicle fuel evaporation control system [2]. The system uses the adsorption and desorption of activated carbon in the activated carbon canister to recover and reuse fuel vapor. On the one hand, it can prevent fuel evaporative pollutants from being released into the atmosphere, on the other hand, the recovery of fuel
vapor can save energy.

In the vehicle fuel evaporation control system, the activated carbon canister is the core component and plays a vital role in the performance of the entire system. The adsorption and desorption performance of the canister should be considered at the same time in the design of the canister. Only when these two performances are both achieved, the performance of the entire system can be optimized. The distribution of the flow field in the canister plays an important role in the adsorption and desorption performance of the canister [3,4]. Another determinant of the adsorption performance is the type of the activated carbon inside. The activated carbon could be produced from coal, wood, coconut shell, etc. The pore size distribution in different types of activated carbon is different. The fuel vapor is mainly absorbed by the micropores (<150nm) and mesopores (150~20000nm) in the activated carbon [5]. In addition, the size and the shape of the carbon particles will also affect the ability to adsorb fuel vapor [6].

Since the design of activated carbon canisters involves the processes of gas flow, adsorption and desorption in the active carbon layer, the numerical simulation analysis using computational fluid dynamics (CFD) methods has become an effective mean to guide the design and optimization of the activated carbon canister. Hou et al. [7] established a computational domain model of an automobile activated carbon canister, simulated the internal structure of active carbon with porous media, and analyzed the internal flow field of the canister under the adsorption and desorption conditions. Li et al. [8] analyzed the influence of the atmosphere orifice on the flow resistance in the canister during the adsorption and desorption process. Zhai et al. [9] conducted a numerical simulation study on the adsorption and desorption process at a certain flow rate for an activated carbon canister used in onboard refueling vapor recovery (ORVR) system, analyzed the velocity field, pressure distribution, and summarized the internal flow characteristics of the canister. Sato et al. [10, 11] used CFD methods to evaluate the adsorption and desorption performance of butane in carbon canisters. Bai et al. [12,13] used the CFD method to model the internal flow of the carbon canister, and developed a user-defined function (UDF) to reflect the adsorption/desorption process of the activated carbon canister.

In this paper, a numerical simulation of the internal flow and the adsorption process of an activated carbon canister used in an ORVR system was carried out to analyze the influence of the structure of the canister on the flow distribution and the adsorption process.

2. CFD simulation

2.1 Geometry model and grid generation
The numerical simulation was aimed at an activated carbon canister that met the requirements of the ORVR system. The appearance of the canister was shown in Figure 1. The amount of the activated carbon in the canister was 2L. MeadWestvaco BAX-1500 type active carbon was used. Its material properties were shown as Table 1.

The software Gambit was used to generate the grid model (see Figure 2). A hexahedral grid was used, the main grid size was 2mm, and the grids were refined to 1mm for each pipe and narrow parts. The total number of grids was about 800,000.
2.2 Boundary conditions and solver setup

The numerical simulation used the software Fluent to model the transient flow in the activated carbon canister. The upwind second-order difference scheme was used to discrete the N-S equations. PISO was used for pressure-velocity coupling as it is very suitable for the transient simulation. The activated carbon filling area in the calculation domain adopted a porous media model, where the viscous resistance coefficient $1/\alpha = 4.2313 \times 10^{-8}$, and the inertial resistance coefficient $C_2 = 33692.9$. The Dubinin-Astakhov adsorption model [14] was added to Fluent through UDF to simulate the adsorption of the butane. The model was proposed by Dubinin et al. based on the theory of volume filling of micropore (TVFM). It was widely used to describe microporous adsorbents.

According to the evaporative pollutant emission test regulations in China 6, in the adsorption process of the canister, the fluid material to be adsorbed was a mixture of 50% butane (C4H10) and 50% nitrogen (N2) by volume, and the mass flow rate of butane was 40g/h. In the desorption process, the compressed air was introduced from the atmosphere orifice at a volume flow rate of 25L/min. The inlet boundary velocity could be obtained by calculation. The specific boundary condition settings were shown in Table 2. The simulation time was set to 12000s.

| Table 2. Boundary conditions |
|-------------------------------|-----------------|
| **Computational domain**     | **Adsorption process** | **Desorption process** |
| initialization               | Air, temperature: 293K, pressure: 0Pa (gauge pressure) | 50% C4H10 and 50%N2, temperature: 293K, pressure: 0Pa (gauge pressure) |
| **Working fluid at the inlet** | 50% C4H10 and 50% N2 | Air |
| **Velocity /Temperature at inlet** | 0.078m/s /293K (adsorption orifice) | 3.812m/s /293K (atmosphere orifice) |
| **Turbulence**                | 0.01/0.0012m     | 0.06/0.0012m     |
3 Results and discussion

3.1 Flow field distribution in activated carbon canister during adsorption/desorption process

![Figure 3. Pressure distribution in adsorption process](image)

![Figure 4. Velocity field distribution in adsorption process](image)

It could be seen from the pressure distribution of the adsorption process in Figure 3 that the pressure gradient in the activated carbon canister during the adsorption process was not obvious due to the relatively low adsorption flow rate. The pressure on the adsorption orifice was the highest, and the pressure gradually decreased as it moved away from the adsorption orifice. The pressure difference between the adsorption orifice and the atmosphere orifice was only about 30Pa.

From flow field distribution in Figure 4, it could be seen that the mixed gas flowed in from the adsorption orifice of the carbon canister and flowed out from the atmosphere orifice. The areas with high velocity were mainly located in the adsorption orifice and the atmosphere orifice area, and the flow rate was about 0.1~0.17m/s. Since the cross-sectional area of the activated carbon layer area had been greatly increased, and the porous medium simulated activated carbon area had a certain flow resistance, the velocity through the activated carbon layer was reduced and only about 0.001m/s, which belonged to laminar flow. This was conducive to the full absorption of butane by the activated carbon.

Figure 5 showed that the pressure distribution in the carbon canister during the desorption process. Because the desorption flow rate was higher than the adsorption flow rate, the whole activated carbon canister had obvious pressure gradient distribution. The maximum pressure was located at the atmosphere orifice (inlet) and the minimum pressure was located at the desorption orifice (outlet). The pressure difference between the two locations reached about 900Pa.

It could be seen from Figure 6 that in the entire flow field area of the canister, the area with higher velocity was mainly located in the atmosphere orifice and the desorption orifice area. The flow velocity at the atmosphere orifice was about 4m/s, and the flow velocity at the desorption orifice could reach 10m/s. While the flow velocity in the activated carbon layer area was lower obviously, only about 0.05-0.09m/s due to the flow resistance in the activated carbon layer.
3.2 Butane concentration distribution in the adsorption process

Figure 7 showed the distribution of the mass fraction of C4H10 adsorbed by the canister at different times. In the initial adsorption stage, due to the high inlet velocity and the high gas flow momentum, the concentration distribution was non-uniform, and the activated carbon under the inlet saturated faster than other positions. However, as the adsorption progressed, the concentration distribution gradually became uniform, and the butane concentration in the canister advanced toward the atmosphere orifice evenly.

3.3 Thermal effect from adsorption and adsorption capacity of carbon canister

In the adsorption process, gas molecules move to the solid surface of the activated carbon, and their movement will be greatly reduced, so heat will be released. The heat generated in the adsorption process is the adsorption heat [15]. In order to monitor the temperature changes of different positions in the canister during the adsorption process, the monitor points selected on the middle section of the canister were shown in Figure 8.
It could be seen from Figure 9 that the temperature of each monitor point had basically the same changing trend over time, and all had gone through a process of first increasing and then decreasing. This was because the adsorbed molecules were first adsorbed on the adsorption sites of the activated carbon with higher potential energy. This process was accompanied by a large amount of heat release due to the larger potential energy difference. When the adsorption sites with higher potential energy were filled, the adsorption occurred at the adsorption site with lower potential energy, and the heat released gradually decreased [5]. When the heat taken away by the gas through the activated carbon bed was greater than the heat released during the adsorption process, the activated carbon bed temperature gradually decreased.

Figure 9 showed that the temperature of monitor point 3 was the highest in each time. This was mainly because the monitor point 3 was located in the center of the canister, and the thermal conductivity of the activated carbon was low, so that the heat could not be transferred out in time. The temperature of monitor point 1 did not change much and close to the temperature of the gas flow. This was because the monitor point 1 was near the inlet, where the thermal convection was relatively intensive, and the generated adsorption heat could be taken away faster by the flow. The lower temperature at the monitor point 6 was mainly because the monitor point 6 was close to the wall surface of the canister. Therefore, the heat transfer was accelerated through the heat conduction to the canister wall and the heat convection between the wall outside and the environment.

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4. Conclusions

In this paper, a numerical simulation of the internal flow and the adsorption process of an activated carbon canister used in an ORVR system was conducted to analyze the influence of the structure of the canister on the flow distribution and adsorption process. The main conclusions are as follows:

(1) In the adsorption process, the flow velocity through the activated carbon layer was only about 0.001 m/s, which belonged to laminar flow. This was conducive to the full absorption of the butane by the activated carbon. In the desorption process, the pressure difference between the atmosphere orifice and the desorption orifice reached about 900 Pa. The flow velocity distribution in the activated carbon layer area was uniform, and the desorption flow velocity reached 0.05-0.09 m/s. The higher flow velocity was beneficial to the desorption of the activated carbon.

(2) In the initial adsorption stage, due to the high flow velocity through the inlet, the butane concentration distribution was non-uniform, and the activated carbon under the inlet saturated faster than other positions. However, as the adsorption progressed, the concentration distribution gradually became uniform, and the butane concentration in the canister advanced toward the atmosphere orifice evenly.

(3) The activated carbon released heat during the adsorption process. The temperature at each monitor point showed a trend of fast increasing first and then slowly decreasing. The temperature at the monitor point in the middle of the canister was the highest, while the temperature near the canister wall and the adsorption orifice was lower.

(4) The adsorption capacity of each monitor point increased significantly in the early stage of the adsorption process, while in the later stage tended to be stable. The adsorption capacity of butane by the activated carbon was directly affected by the temperature of the activated carbon layer. The higher temperature was not conducive to the adsorption process.

Acknowledgements

The study was financially supported by the Open Fund of the National Engineering Laboratory for Mobile Source Emission Control Technology (No. NELMS2017B07), the Scientific Research Project of Tianjin Municipal Education Commission (No. 2017KJ114) and the Talent Start Project of Tianjin University of Technology and Education (No. KYQD14050)

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