A CFD pressure drop model for microfibrous entrapped catalyst filters using micro-scale imaging

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A micro-scale pressure drop model for microfibrous entrapped catalysts (MFEC) is constructed based on experimental scanning electron microscope (SEM) images using computational fluid dynamics (CFD). This model investigates the separate contributions of fibers, entrapped particles, particle shape factors and the compressibility of MFEC to the total pressure drop in a high air velocity condition. A theoretical calculation is conducted to determine the flow type within the MFEC. Top view and side view SEM images of MFEC are taken to reproduce their 3D geometric structure, which significantly improves the accuracy of the model compared with other simplified models. Volume loading of fibers and entrapped particles, as well as media compressibility, are found to be major contributors to pressure drop. In an effort to reduce pressure drop, two types of leading-edge/trailing-edge filter fairings are also studied. Triangle fairings added to the leading edge and trailing edge of MFEC decrease pressure drop, especially at higher face velocities.

Keywords: pressure drop; computational fluid dynamics (CFD); scanning electron microscope (SEM); microfibrous entrapped catalysts (MFEC)

1. Introduction

Molecular filtration needs have increased dramatically due to demand for high-quality air in working and residential areas. The typical solution to meet these demands is to adapt traditional reactors such as packed beds or monoliths, even though they were originally intended for very different purposes. For such un-optimized adaptations, certain issues influence the performance of the reactors. Packed-bed reactors generally have higher gas-solid mass transfer rates than the monolith reactors. However, these reactors have comparatively low voidage, which leads to a high pressure drop penalty, especially under high velocity conditions. Monolith reactors, which offer a comparatively lower pressure drop, suffer from low gas-solid transfer rates. This translates to larger reactors that require more catalysts. With these issues in mind, a new class of structure, which offers both high voidage and gas-solid mass transfer rate, is needed for high velocity applications.

Microfibrous entrapped catalysts (MFEC) were first developed at Auburn University. They are a sinter lock structure of metal fibers which is manufactured via a conventional high-speed paper-making process. This material shows good structural stability, high thermal conductivity, and high contact efficiency (Cahela & Tatarchuk, 2001; Harris, Cahela, & Tatarchuk, 2001; Kalluri, Cahela, & Tatarchuk, 2009; Kalluri, Duggirala, Cahela, Roy, & Tatarchuk, 2008; Karwa & Tatarchuk, 2012). However, the biggest advantage of MFEC over packed beds and monoliths is their reduced pressure drop. Sothen and Tatarchuk (2008, 2009) have established a semi-empirical model to predict pressure drop over pleated MFEC, while attempts have been made by Rivers and Murphy (2000) to study pressure drop for similar materials. Caesar and Schroth (2002) and Chen, Pui, and Tang (1996) have studied the mechanical structure of filter design on pressure drop. No model has been constructed to study the pressure drop of pleated structures at a micro-scale level, which is supposed to be able to analyze the importance of fibers, particles and voidage in pressure drop. This is due to the large difference between the scale of fibers and entrapped particles to that of the filter.

The objective of this research is to establish a 3D computational fluid dynamics (CFD) model based on scanning electron microscope (SEM) images of the fibrous media. This model is based on the hypothesis that the pressure drop across a small cross-sectional area of the media is identical to the overall pressure drop of the media at high velocity (Dhandapani & Oyama, 1997; Kameya & Urano, 2002). The hypothesis is proved by a numerically obtained velocity profile within the media. Different MFEC media are investigated to compare the separate contribution of fibers, particles, shape factor and media compressibility to overall pressure drop. Furthermore, pressure drop across a pleated filter is determined based on the micro-scale simulation results. The resulting model provides design parameters for filters under high velocity conditions.

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2. Materials and methods

2.1. Flat MFEC pressure drop measurement

The high volumetric flow test set-up is shown in Figure 1(a). This closed-loop setup (6" diameter) includes a 40 horsepower blower (Fan Equipment Company Inc.) to circulate air at high face velocities (10–40 m/s). Temperatures are recorded at different locations (blower outlet, elbows, reactor upstream, reactor downstream and blower inlet) on the loop using Omega® J type thermocouples. Pressure drop across the media is recorded using IDP10-T differential pressure transmitters. Two media have been tested for pressure drop: 8 μm diameter nickel fiber sheet with a thickness of 2.5 mm, and media entrapped with 150–250 μm alumina particles with a thickness of 4 mm. Samples are clamped using a wide-edge (2") flange to minimize the housing effect on the pressure drop. Each sample is tested three times with increasing and decreasing air velocity; the results are then averaged. No pressure drop difference is seen among repeated tests. A metal wire mesh is used as downstream support for the microfibrous material; the background resistance of the mesh is measured with the same method and deducted from the total pressure drop. System speed is acquired by calculating the pressure drop across a bare section on the rig and verified by a Dwyer® 1/8" stainless steel pitot tube at different temperatures. Figure 1(b) shows the heat balance in the system. The system is constructed as a closed loop due to the difficulty of simulating turbine bleed air temperature using a common blower. The skin friction on the pipe wall brings up the system temperature quickly at high face velocities. When the system is running at relatively lower face velocities, six 1800 W ring heaters assist with heating. In addition, the loop is insulated with 2" thick mineral wool. By balancing all the heating sources, the system can be controlled between 100 and 200°C, which is in the operating range of turbine bleed air. The air humidity level during the pressure tests are not a concern due to the high temperature.

2.2. Micro-scale images of MFEC

The challenge of this model is to determine the geometry of the fibers and entrapped particles for simulation. Since the ratio of the reactor size to the fiber size is exceptionally large, drawing and meshing the actual reactor with fiber details is not possible. The MFEC material is made by a wet-lay process, which guarantees that the fibers and particles are randomly dispersed. Therefore, the structures for simulation are drawn based on a randomly selected area of the MFEC. This method is also supported by the velocity profile calculations in section 3. Only a few top MFEC layers are visible and easy to distinguish from one another, so the drawing of the fiber media structure by SEM images is based on these layers. As to the inner layers, duplicates of the top layers are used, because all layers are randomly dispersed and assumed to be similar in performance.

Another aspect to consider when sketching the geometry is media thickness. Since fibers are randomly dispersed and vary in shape, the actual media thickness is much greater than the sum of single fiber thicknesses. SEM images have been taken of the side of the material to estimate the average fiber thickness in the axial direction. As indicated in Figure 2, the average number of fiber layers for a given thickness of media is similar. The SEM image shows an average of 10–11 layers for 280 μm thickness of media. Layers are isolated 30 μm apart from each other for the actual modeling. Since only a small area of the microfibrous surface has been isolated to simulate pressure drop, sampling from different spots of the MFEC has been tested for geometry dependence. Each CFD geometry is drawn to closely imitate the real SEM images, while the volume loading of fibers is controlled according to the original specification from which the fiber sheets are made. The volume loading of fibers is controlled by adjusting the media depth to match that of the MFEC tested. For blank simulation, particles are disassembled from the previous drawings and adjusted for volume loading. The

![Figure 1. High face velocity test setup: (a) schematic of the test setup and (b) heat balance of the system.](image-url)
particle effect on the pressure drop is observed without any disturbance from fiber geometry.

3. Results and discussion

3.1. Flow pattern in media flow

The pipe Reynolds number that corresponds to a 10–40 m/s flow is \( \sim 10^5 \), indicating turbulent flow. However, the intra-bed Reynolds number is only 455–1818 in the MFEC because of the smaller characteristic length of the fibers. The intra-bed Reynolds number can be calculated using the dimension of fibers (\( \sim 10 \mu m \)), particles (\( \sim 100 \mu m \)) or the void (\( \sim 100 \mu m \)). The intra-bed Reynolds number is significantly smaller than the pipe Reynolds number no matter which characteristic length is used, which leads to different flow types. The Reynolds number calculation is reported using fiber size in this research. When the intra-bed Reynolds number is in the transition region, the flow pattern has to be determined according to specific operating conditions. Hill and Koch (2002) have studied the transition from steady to weakly turbulent flow in a close-packed ordered array of spheres. It is shown that at an intra-bed Reynolds number of approximately 30, the development of a vortex begins and the transition to unsteady flow occurs. At an intra-bed Reynolds number of approximately 50, further unsteady flow develops. After this region, the velocity fluctuation becomes more isotropic and can be treated as a turbulent flow. Since the intra-bed Reynolds number in this application is well over 50, the flow within the porous media is treated as turbulent in all simulations. In addition, Kolmogorov’s micro-scale is analyzed for the turbulent flow in the bed. Patil and Liburdy (2013, 2015) found that the pore characteristics are similar from pore to pore for high Reynolds number flows. Scaling based on bed-averaged variables like characteristic length and inlet face velocity characterize the Kolmogorov’s scale, despite very different mean flow conditions.

3.1.1. Velocity profile in 6” flat microfibrous material

Darcy’s law is used for pressure drop in the low face velocity region (Angirasa, 2002; Vafai & Tien, 1981). This equation is invalid for higher velocity applications. Rivers and Murphy (2000) have linked this deviation to fiber compression by inertial forces. Forchheimer law, an extension of Darcy’s law, has been widely used in these situations to account for the nonlinear deviation. Various approaches have been attempted by Chen et al. (1996), Rivers and Murphy (2000) and Caesar and Schroth (2002) to determine a universal equation that predicts the constants in Forchheimer law. Though all methods have generated accurate results for certain applications, no valid prediction can be made based only on fiber dimension, voidage, particle dimension and other basic properties of the fiber material. A mass conservation equation and a Navier-Stokes equation for porous media developed by Vafai and Tien (1981) are used to calculate the velocity profile in this study. The Knudsen number is calculated to validate using the Navier-Stokes equation at the scale used in the research. The result shows that the Knudsen (\( \lambda/D \)) number (0.00053) is far less than 0.1, and thus it is valid to use the Navier-Stokes equation (Hadjiconstantinou, 2006). Theoretical calculations of flow in microfibrous media are done by solving the volume-averaged Navier-Stokes equation, which is simplified by the operating conditions in this research. Simplification in the flow-wise direction is made by assuming the radial and angular velocity to be zero. This is because the face velocity in the flow-wise direction is much higher than in the other directions. Terms containing radial and angular velocity can be neglected. A similar equation can be acquired for the radial direction. The boundary conditions used for the calculation are as follows: an incoming air velocity of 10 m/s; a non-slip condition is used at the wall; and the flow-wise velocity does not change when coming out of the trailing edge of the media or at the center of media.

3.1.2. Numerical process

The partial differential equation (PDE) is discretized using a central difference formulation and integrated by a first-order Euler explicit method. The final results are generated based on uniform grid spacing using 600 divisions in the radial direction and 20 in the axial direction, due to the physical shape of the test media (6” diameter, 4 mm thickness). The domain is also meshed, with 700 divisions in the radial direction and 30 in the axial direction, for the grid dependence test. Both are calculated to steady state based on the same error estimate (least square error estimate with a limit of \( 10^{-5} \)), and the final results are identical. A Von Neumann stability analysis was performed for the PDE, indicating that the scheme is conditionally stable for a Courant number of less than 0.5. The velocity profiles in the microfibrous material are shown in Figure 3(a). Figure 3(b) shows the velocity profile near...
the boundary. The flow type within the MFEC is a plug flow. The boundary layer accounts for less than 3% of the total area. This means that the average velocity is identical in most of the fiber sheet area. It is determined that the total pressure drop of a flat sheet is the sum of the pressure drop across any selected slice disassembled from the flat sheet. This supports the method used in drawing the 3D MFEC structure in section 2.2. Random areas are tested to avoid positional dependence in the pressure drop.

3.2. Pressure drop for micro-scale MFEC with and without entrapped particles

At 200°C and atmospheric pressure, the air density is 0.75 kg/m³ and the kinetic viscosity is $3.5 \times 10^{-5}$ m²/s. The air was treated as non-compressible fluid in the simulations. Different turbulence models were attempted in the simulation process; the $k-\varepsilon$ turbulence model was used in ANSYS Fluent simulations (ANSYS Fluent, 2013; Computer: 8G memory; 100 ~ 120 iterations for each simulation) due to
the relatively low face velocity in the bed (Combest, 2012). The velocity was simulated using the second-order upwind method in Fluent with a finite volume method, and the outlet pressure was set at 1 atm. Since this simulation only represents a disassembled part of the 6" media sheet, all boundaries for the simulation were set to be symmetric, so that no wall effect was shown for the pressure drop. The pressure drop across a blank 8 μm nickel fiber was simulated first. The fiber material used was 1.2% volume loading. The distance between fibers was determined by side-view SEM images of the MFEC. The simulation domain consisted of four unit cells (Figure 4(a and b)), which are 1.1 mm in length. Since 4 mm media are used in pressure drop tests, pressure drop per thickness of media was used to compare the experimental and simulation data. Figure 4(b) shows a simulation of the pressure drop across fibrous media with an inlet velocity of 10 m/s and a total pressure drop of 2750 Pa/mm. The simulation result is compared with the experimental result in Figure 5. Both the experiment and simulation show a quadratic pattern of pressure drop at high velocities, which is consistent with Forchheimer law. However, the simulation results show a deviation from the experimental data that grows with increasing velocity. The deviation is expected because the MFEC is under compression due to the pressure difference between the leading edge and trailing edge. This effect will be examined in a later section of this study, which serves to increase the accuracy of this pressure drop model. This comparison between experiment and simulation is based on a randomly-selected area of the MFEC, as described in section 2.2. Three more randomly-selected areas were also simulated using the same boundary conditions to test the fiber position dependence of pressure drop. No obvious deviation was seen among these simulations.

Since the volume loading of particles in entrapped fiber sheets is much higher than the fiber itself, the entrapped particles contribute to a large portion of the total pressure drop. Typically, volume loading of particles ranges from 20–30% for MFEC. For this application, the particle volume loading is 20% and the particle size is controlled at 150–250 μm. The particles are assumed to be ideal in shape (spherical) and average in size (200 μm) in the simulation. Figure 6 shows an SEM image of particle-entrapped fiber media, which is drawn in Figure 4(c) as a simulation unit cell. The same boundary conditions are adopted in the previous simulation to avoid an unfair comparison. Bare sections are left both upstream and downstream within the simulated area so that flow can be fully developed before entering the fibers and immediately after exiting the fibers. Figure 4(d) shows the simulation using a round particle. The inlet velocity is 10 m/s and the total pressure drop is 3750 Pa/mm. Deviation is still present in this case due to the media compressibility.

The real entrapped particles, visually investigated in SEM images, are not spheres. Karwa and Tatarchuk (2012) have empirically obtained shaped factors of entrapped particles using the Blake Kozeny equation for MFEC (Table 1). In this research, 180–210 μm particles are used and a shape factor of 0.8 is chosen. Close investigation of SEM images of the particles reveals that the shape of

![SEM image of particle-entrapped fiber media](image_url)

**Figure 6.** SEM imaging of an entrapped particle microfibrous sheet surface (8 μm fibers and 150–250 μm alumina particles entrapped).

| Particles/fibers | Shape factors | Solid fraction during measuring |
|------------------|---------------|--------------------------------|
| 90–125 μm particles | 0.77 | 0.62 |
| 180–210 μm particles | 0.80 | 0.62 |
| 500–600 μm particles | 0.74 | 0.62 |
| 4 μm fibers | 1.09 | 0.39 |
| 8 μm fibers | 1.09 | 0.41 |
| 12 μm fibers | 1.04 | 0.40 |
particles is in great approximation to a sphere, only sharp at two ends in most cases. This shape is best simulated with an ellipsoid. The sphericity (Equation 1) and volume (Equation 2) equations are solved for the dimension of the ellipsoid, assuming that the particle volume remains unchanged:

\[ \Phi = \frac{\pi^{1/3} (6V_p)^{2/3}}{A_p} \]

\[ = \frac{2\sqrt{ab^2}}{a + \left(\frac{b^2}{\sqrt{a^2 - b^2}}\right) \ln \left(a + \sqrt{a^2 - b^2}/b\right)} \]  

(1)

\[ V = \frac{4}{3} \pi ab^2. \]  

(2)

With the same volume loading of particles as round particles and a shape factor of 0.8 for entrapped particles, the calculated results for the ellipsoid are 206 μm for \(a\) and 69 μm for \(b\). The alignment of the ellipsoid particles is determined by several factors, including the media preparation process, particle volume loading and post compression of the media. The samples used in this research were prepared by wet lay process with modified fluid viscosity; due to gravity, the particles were preferably aligned in the direction perpendicular to the flow. In addition, the samples were pressed to the same thickness before pressure drop tests, which helped with the consistency of particle alignment. Therefore, the preferable alignment direction is used in this simulation. The drawing for the simulation is shown in Figure 4(e). The fiber layout of the elliptic particle unit cell is the same as that for fiber only and fiber with round particles. The boundary conditions are also the same, with bare sections attached upstream and downstream. According to the Blake Kozeny equation, the expected pressure drop for lower shape factor particles will be higher due to the shape irregularity. Figure 4(f) shows a sample simulation of pressure drop across fibrous media with elliptic particles. The inlet velocity is 10 m/s and the total pressure drop is 4250 Pa/mm. All three simulation results are compared in Figure 7. It is shown that the elliptic simulation result is better in approximating the experimental result, which is consistent with the Blake Kozeny equation. However, deviation from fiber compressibility still exists for elliptic particle simulation.
Figure 9. Pressure drop for fiber-only with adjusted material thickness (fiber volume loading 1.25%).

Figure 10. Pressure drop for fiber with elliptic particles with adjusted material thickness (fiber volume loading 1.25%, particle volume loading 20%).

Table 2. $R^2$ value by compressibility adjustment for fiber-only and entrapped particles simulations.

|                     | Constant thickness | Adjusted thickness |
|---------------------|--------------------|--------------------|
| Fiber-only sheet    | 0.784              | 0.989              |
| Sheet entrapped with round particles | 0.095 | N/A |
| Sheet entrapped with elliptic particles | 0.714 | 0.999 |

3.3. MFEC compressibility

Volume loading of different components substantially changes the pressure drop across a fiber material. When tested at high face velocities, the pressure difference between the leading edge and trailing edge of the fiber...
material compresses the fiber material. This compression causes a temporary volume loading change on the fibers and other entrapped components. To take these effects into consideration, fiber thickness is tested at different pressures. Wang, Kim, Lee, and Kim (2008) have suggested that fiber thickness is a linear function of applied pressure. The media thickness test results are shown in Figure 8. Linear dependence is observed both for fibers with and without entrapped particles. It is shown that the media compresses up to 20% in thickness under the operating conditions. However, the pressure ($\sim 10^5 \text{ Pa}$) is still in the elastic compression range of the media. No particle crushing or permanent shape change of the media is involved in the compression process. The volume loading changes were applied to a fiber-only case and a fiber with entrapped particle case. The simulations in the previous section were repeated, with media compression taken into account (Figures 9 and 10). Due to the corrections of the volume loading of fibers and entrapped particles, the pressure model accuracy was improved dramatically, especially at higher face velocities. For the fiber-only case (Figure 9), the adjusted thickness pressure drop shows good consistency with the experimental result. Table 2 compares the coefficients of determination before and after the thickness adjustment. For the entrapped particles cases (Figure 10), a similar improvement in simulation accuracy is found when taking into account media compressibility. The shape factor contribution of the particles to the total pressure drop can be distinguished by comparing the experimental results and round particle simulation. Since the volume loading of fibers in the media is relatively small and the shape factor of fibers is close to one in most cases, shape factor is not considered for the fibers in this simulation.

3.4. Pressure drop for pleated MFEC

The previous analysis using micro-scale images precisely predicts pressure drop for certain compositions of fibers and particles at high pipe Reynolds numbers. As mentioned in the previous section, the gigantic difference in the dimension of pleat structure and fibers makes it impossible to simulate the pressure drop for the whole filter structure using computational methods (MFEC defined as porous media in Fluent). However, a quadratic form of pressure drop (Forchheimer law) curve was obtained for each fiber sheet in both the simulation and the experiment. This curve can be used to predict pressure drop in the porous media in filter simulations. In this way, the dimension difference is treated by simulating the same porous media in both micro and macro scope. It is important to note that this method is only valid for high pipe Reynolds numbers, where the average face velocity profile resembles a plug flow. In high volumetric flow tests, the microfibrous media was engineered into a pleat structure to reduce the pressure drop. These structures help with the reduction of the amount of air going into each of the pleats. The pressure drop and velocity profile for these complex structures are simulated using previous flat sheet simulation results. In addition, pleat tips increase the total pressure drop. Fairings added to the pleat tips have been tested experimentally and by simulation using Fluent to understand the benefit.

Figure 12. Filter structures (top row) and comparison between simulation and experiment (bottom row) for pleated MFEC (A and B, 9" deep), MFEC with triangle fairings (C and D, 6" long) and MFEC with round-top fairings (E and F, 6" long).
of these fairings. A second-order upwind method was used in the simulation. All cases were simulated as single solution rather than parallel solutions. The inlet velocity in the simulation was in the range of 10–40 m/s. The outlet pressure at downstream of the fiber media was atmospheric. The calculations converged at $10^{-4}$ for velocities, continuity, $k$ and epsilon. The iterations for no fairing, round-top fairings and triangle fairings were 105, 114 and 124 respectively. Figure 11 shows the pressure drop simulations for pleat MFEC, MFEC with triangle fairings and MFEC with round-top fairings and their corresponding velocity contours. Figure 12 shows the filter structure for the pressure drop test experiment and the comparison between measurements and simulation. Figure 13 compares the pressure drop reduction by adding round-top and triangle fairings to the pleat tip. It was found that the total pressure drop is affected by how fast the air is compressed near the pleat tip area. The triangle fairings gradually compress the air, and round top fairings only perform a little better in pressure drop compared to no fairings, because only the leading edge of the fairings is effective in gradually compressing air. Structures with proper fairings have been proven to reduce the total pressure drop by up to 15%.

The amount of energy required to push the air through the filter is defined as the product of volumetric flow rate, pressure drop and operation time. As the pleat number changes, pressure drop is significantly affected. There exists an optimum pleat number for each structure because the pressure drop switches between the media-dominant regime and geometric-dominant regime. Figure 14 shows the simulated results for different pleat structures. The pressure drop for structures with a low pleat number ($< 5$) was simulated and tested experimentally. The pressure drop for structures with a higher pleat number ($> 4$) was simulated. The optimum pleat number for this specific structure was found to be 4 (W structure).

4. Conclusion

A pressure drop model for pleated microfibrous media has been established by considering the micro-scale structure of the material. SEM images for the top and side of microfibrous media were obtained to determine the structure of the fibers for simulation. The pressure drops were modeled for fiber material only and fiber with entrapped particles, showing the significant contribution of the entrapped particles to the pressure drop. The shape factor effect of the entrapped particles was also investigated and found to improve the model accuracy. Due to the malleable nature of the metal fibers, they can be temporarily compressed when a pressure difference exists between the leading edge and trailing edge. This effect contributes to higher volume loading of both the fiber and the particles. Simulations based on corrected volume loading were conducted. Both blank and entrapped MFEC simulations showed improved consistency with experimental results when taking media compression into account. The pleat structure pressure drop of the MFEC was simulated based on flat media simulation results. Fairings were added to the pleat tip, demonstrating that triangle fairings help to reduce the pressure drop. The optimum pleat number was also determined for pleated MFEC using computational methods; for the lowest pressure drop, it was found that 4 pleats is optimum.

For a fiber media applied at high velocity conditions, pressure drop across the media is an important factor because it is directly related to operating cost. This model provides a unique solution for obtaining design parameters for fiber media used in various situations. The only parameter in the model that needs experimental determination is the particle shape factor. As the model showed high accuracy in analyzing the contribution of different factors to the
pressure drop, further modification and analysis – including fiber shape factor, fiber diameter, particle diameter, particle orientation, and system pressure – will potentially provide a better understanding of MFEC applications in chemical and physical processes.

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Nomenclature

A | dimensional constant
Ap | surface area (m²)
a | semi major axis length
B | dimensional constant
b | semi minor axis length
D | characteristic dimension (m)
i | grid index
j | grid index
K | media permeability
L | channel length (m)
n | time index
p | pressure (Pa)
Q | volumetric flow rate (m³/s)
r | radius (m)
Re | Reynolds number
t | time (s)
u | average velocity inflow direction (m/s)
V | mass average velocity (m/s)
Vp | volume (m³)
z | axial direction

Greek letters

ε | voidage
ρ | density
λ | mean free path (m)
μ | viscosity (kg/ms)
Φ | shape factor

Subscripts

x | x direction
y | y direction
z | z direction
m | mean
θ | θ direction

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