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POWER LOSS IN MULTISCALE MASS TRANSFER

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ABSTRACT

The power loss is calculated by a multiscale approach in the pressure driven mass transfer in a micro slit pore where there are the physical adsorbed layers respectively on the coupled walls and intermediate between them is a continuum fluid flow. The flow factor approach model for nanoscale flow is taken to simulate the flow of the adsorbed layer, and conventional hydrodynamic flow theory models the continuum fluid flow. The calculation shows that the adsorbed layer on the wall surface can have a very significant effect on the power loss in this multiscale mass transfer, and it can greatly reduce the power loss on the channel owing to heavily reducing the flow rate through the channel because of the strong fluid-wall interaction. In the case of the interfacial slippage on both the wall surfaces, there is a critical power loss in the channel to generate the interfacial slippage, and the power loss on the channel is proportionally increased with the increase of the interfacial slipping velocity, which significantly enlarges the mass flow rate through the channel.

Keywords: *Flow, Mass transfer; Multiscale; Model; Physical adsorption; Power*

1. INTRODUCTION

When the channel height is small enough such as on the scales of 10nm or 100nm, the thickness of the physical adsorbed layer on the wall surface will be comparable to the thickness of the continuum fluid film intermediate between the two adsorbed layers. In this case, the effect of the adsorbed layer on the mass transfer in the channel should be considered, and there should be a multiscale approach to simulate the flows of both the adsorbed layer and the continuum fluid. Multiscale schemes have been proposed a lot for simulating microchannel flows (Atkas et al., 2002; Liu et al., 2007; Sun et al., 2010; Yen et al, 2017). In those multiscale schemes, full atomistic molecular dynamics simulation was used to model the flow of the layer adjacent to the solid surface, and a continuum flow model described the intermediate continuum fluid flow. The obvious shortcoming of them is that it should still take quite long time to carry out molecular dynamics simulation especially for an engineering problem.

In the former research (Zhang, 2019), The author proposed a multiscale approach to the flow in a micro slit pore where the effect of the physical adsorbed layer on the wall surface is considerable and there are the flows of the adsorbed layers and the flow of the intermediate continuum fluid. In this approach, the flow factor approach model for nanoscale flow was used to simulate the adsorbed layer flow, and a continuum flow theory simulated the intermediate continuum fluid flow. This approach has the advantage of fast solving an engineering problem since it gives the closed-form explicit flow equations respectively for the two adsorbed layers and the intermediate continuum fluid.

The present study aims to address on the power loss in a multiscale mass transfer in a micro slit channel by using the multiscale approach proposed by the author earlier. One of the purposes of the study is to reveal the effect of the adsorbed layer on the power loss on the channel in the case of no wall slippage; The second purpose is to reveal the dependence of the power loss on the channel on the interfacial slipping velocity on the wall surface.

2. STUDIED CHANNEL FLOW

Figure 1(a) shows the studied one-dimensional flow in a micro slit pore where the film thickness of the intermediate continuum fluid is so small that the effect of the physical adsorbed layer on the wall surface is considerable. The adsorbed layer should contribute to the flow; If its flow rate is far less than the flow rate of the intermediate continuum fluid, it can be treated as a solid layer; Otherwise, a multiscale model should describe both the adsorbed layer flow and the intermediate continuum fluid flow. The studied channel flow can occur in microporous/nanoporous membrane filtration, microchannel mass transfer and micro bearings et al.. Here, the flow factor approach model for nanoscale flow simulates the adsorbed layer flow and the Newtonian fluid model simulates the intermediate continuum fluid flow. According to the present multiscale approach, the channel flow in Fig. 1(a) is equivalently treated as Fig. 1(b) shows. Here, the interfacial slippage on the channel wall surface is assumed, while the interfacial slippage between the adsorbed layer and the continuum fluid is ignored. Detailed derivations of the three flow equations respectively for the two adsorbed layers and the continuum fluid in Fig. 1(b) have been shown by the author(Zhang, 2019).

3. ANALYSIS

The analysis was primitively developed for a general problem and aimed to be applicable for both asymmetrical and symmetrical multiscale flows in engineering (Zhang, 2019). In the present analysis, it is further assumed that the physical adsorbed layer on the solid surface A is the same with that on the solid surface B in Fig. 1 (b). Thus, $h_{bf,A} = h_{bf,B}$.

3.1 For no interfacial slippage on the channel wall surface

When no interfacial slippage occurs on both the channel wall surfaces,

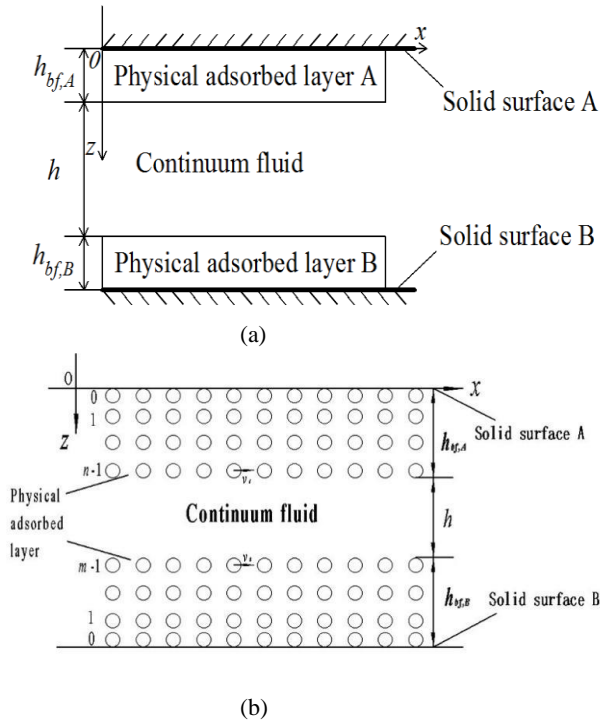[*]*Email:engmech1@sina.com*

(a)

(b)

Fig. 1 The studied multiscale flow in a micro slit pore.

conventional continuum Newtonian flow theory gives the following power loss per unit contact length on the studied slit pore:

$$POW_{conv} = \frac{(\Delta p)^2 (h + h_{bf,A} + h_{bf,B})^3}{12 \eta \Delta l} \tag{1}$$

where Δp is the pressure drop on the channel, Δl is the channel width, η is the fluid bulk viscosity, h is the film thickness of the intermediate continuum fluid, and $h_{bf,A}$ and $h_{bf,B}$ are respectively the thicknesses of the adsorbed layers on the two channel walls.

The present multiscale approach gives the following volume flow rate per unit contact length for either of the adsorbed layers (Zhang, 2019):

$$q_{v,bf} = \left[\frac{F_1 h_{bf,A}^3}{12 \eta_{bf}^{eff}} - \frac{h_{bf,A}^3}{2 \eta_{bf}^{eff}} \left(1 + \frac{1}{2\lambda_{bf}} - \frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n} \frac{\Delta_{n-2}}{h_{bf,A}}\right) \frac{\varepsilon}{1 + \frac{\Delta x}{D}}\right] \frac{\partial p}{\partial x} \tag{2}$$

where $\lambda_{bf} = h_{bf,A}/h$, η_{bf}^{eff} is the effective viscosity of the adsorbed layer and $\eta_{bf}^{eff} = D h_{bf,A}/[(n-1)(D + \Delta_x)(\Delta_l/\eta_{line,l})_{avr,n-1}]$, Δ_x is the separation between the neighboring fluid molecules in the x coordinate direction in the adsorbed layer, $q_0 = \Delta_{j+1}/\Delta_j$ and q_0 is constant, Δ_j is the separation between the $(j+1)^{th}$ and j^{th} molecules across the layer thickness, $\varepsilon = (2DI + II)/[h_{bf,A}(n-1)$ $\cdot (\Delta_l/\eta_{line,l})_{avr,n-1}]$, $F_1 = \eta_{bf}^{eff}(12D^2\psi + 6D\phi)/h_{bf,A}^3$, and n is the number of the fluid molecules across the layer thickness as shown in Fig. 1(b) . Here, $I = \sum_{i=1}^{n-1} i(\Delta_l/\eta_{line,l})_{avr,i}$,

$$II = \sum_{i=0}^{n-2} [i(\Delta_l/\eta_{line,l})_{avr,i} + (i+1)(\Delta_l/\eta_{line,l})_{avr,i+1}]\Delta_i,$$

$$\psi = \sum_{i=1}^{n-1} i(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i} ,$$

$$\phi = \sum_{i=0}^{n-2} [i(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i} + (i+1)(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i+1}]\Delta_i,$$

$$i(\Delta_l/\eta_{line,l})_{avr,i} = \sum_{j=1}^{i} \Delta_{j-1}/\eta_{line,j-1}, and \ i(l\Delta_{l-1}/\eta_{line,l-1})_{avr,i}$$
$$= \sum_{j=1}^{i} j\Delta_{j-1}/\eta_{line,j-1}$$

It gives the following volume flow rate per unit contact length for the intermediate continuum fluid (Zhang, 2019):

$$q_{v,hf} = \left\{-\frac{h^3}{12\eta} + \frac{h^3}{\eta_{bf}^{eff}}\left[\frac{F_2 \lambda_{bf}^2}{6} - \frac{\lambda_{bf}}{1 + \frac{\Delta x}{D}}\left(\frac{1}{2} + \lambda_{bf} - \frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n}\frac{\Delta_{n-2}}{h}\right)\right]\right\}\frac{\partial p}{\partial x} \tag{3}$$

where $F_2 = 6\eta_{bf}^{eff} D(n-1)(l\Delta_{l-1}/\eta_{line,l-1})_{avr,n-1}/h_{bf,A}^2$.

If the effect of the adsorbed layer is considered, the present multiscale approach thus gives the following power loss per unit contact length on the channel:

$$POW = \Delta p(2q_{v,bf} + q_{v,hf}) \tag{4}$$

Define $r_{p,ns} = POW/POW_{conv}$.

3.2 For the interfacial slippage on the channel wall surfaces

When the pressure gradient for driving the flow is sufficiently large, the adsorbed layers will slip respectively on the upper and lower channel wall surfaces and there is the slipping velocity $\bar{u}$ of the adsorbed layers relative to the two channel wall surfaces.

If the pressure driven flow is in the direction from the left-hand side to the right-hand side, when the interfacial slippage occurs on both the wall surfaces, it can be easily derived from the multiscale analysis (Zhang, 2019) that:

$$\frac{\partial p}{\partial x} = -\frac{\tau_s}{\frac{1}{2}h + D(n-1)} \tag{5}$$

where τ_s is the shear strength of the adsorbed layer-wall surface interface and D is the fluid molecule diameter.

In this case, the analysis gives the following total volume flow rate per unit contact length through the channel, which consists of the adsorbed layer flows and the continuum Newtonian fluid flow:

$$q_v = 2\bar{u}h_{bf,A} + \bar{u}h \quad -\left\{\frac{F_1 h_{bf,A}^3}{6\eta_{bf}^{eff}} - \frac{h^3}{12\eta} - \frac{h_{bf,A}^3}{\eta_{bf}^{eff}}\left(1 + \frac{1}{2\lambda_{bf}}\right.\right.$$
$$\left. - \frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n}\frac{\Delta_{n-2}}{h_{bf,A}}\right)\frac{\varepsilon}{1 + \frac{\Delta x}{D}} + \frac{h^3}{\eta_{bf}^{eff}}\left[\frac{F_2 \lambda_{bf}^2}{6} - \frac{\lambda_{bf}}{1 + \frac{\Delta x}{D}}\left(\frac{1}{2} + \lambda_{bf} - \frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n}\frac{\Delta_{n-2}}{h}\right)\right]\right\}$$
$$\cdot \frac{\tau_s}{\frac{1}{2}h + D(n-1)} \tag{6}$$

The power loss per unit contact length on the channel is thus:

$$POW = \frac{\tau_s \Delta l}{\frac{1}{2}h + D(n-1)}\left\{2\bar{u}h_{bf,A} + \bar{u}h - \left[\frac{F_1 h_{bf,A}^3}{6\eta_{bf}^{eff}} - \frac{h^3}{12\eta} - \frac{h_{bf,A}^3}{\eta_{bf}^{eff}}\right.\right.$$
$$\cdot \left(1 + \frac{1}{2\lambda_{bf}} - \frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n}\frac{\Delta_{n-2}}{h_{bf,A}}\right)\frac{\varepsilon}{1 + \frac{\Delta x}{D}} + \frac{h^3}{\eta_{bf}^{eff}}\left[\frac{F_2 \lambda_{bf}^2}{6} - \frac{\lambda_{bf}}{1 + \frac{\Delta x}{D}}\left(\frac{1}{2} + \lambda_{bf}\right.\right.$$
$$\left.\left.\left. - \frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n}\frac{\Delta_{n-2}}{h}\right)\right]\right\}\cdot \frac{\tau_s}{\frac{1}{2}h + D(n-1)}\right\}$$
$$= \frac{\tau_s \Delta l (2h_{bf,A} + h)\bar{u}}{\frac{1}{2}h + D(n-1)} + POW_{cr} \tag{7}$$

where POW_{cr} is the critical power loss per unit contact length on the channel initiating the interfacial slippage on the wall surface and it is expressed as:

$$POW_{cr} = -\frac{\tau_s^2 \Delta l}{\left[\frac{1}{2}h + D(n-1)\right]^2}\left\{\frac{F_1 h_{bf,A}^3}{6\eta_{bf}^{eff}} - \frac{h^3}{12\eta} - \frac{h_{bf,A}^3}{\eta_{bf}^{eff}}\left(1 + \frac{1}{2\lambda_{bf}}\right.\right.$$
$$\left. - \frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n}\frac{\Delta_{n-2}}{h_{bf,A}}\right)\frac{\varepsilon}{1 + \frac{\Delta x}{D}} + \frac{h^3}{\eta_{bf}^{eff}}\left[\frac{F_2 \lambda_{bf}^2}{6} - \frac{\lambda_{bf}}{1 + \frac{\Delta x}{D}}\left(\frac{1}{2} + \lambda_{bf} - \frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n}\frac{\Delta_{n-2}}{h}\right)\right]\right\} \tag{8}$$

The power loss difference from the critical power loss is:

$$\Delta POW = POW - POW_{cr} = \frac{2\tau_s \Delta l \bar{u}}{1 - r_0} \tag{9}$$

where

$$r_0 = \frac{2\left(\frac{q_0 - q_0^n}{q_0^{n-1} - q_0^n} \frac{\Delta_{n-2}}{D} + 1\right)}{1 + 2\lambda_{bf}} \frac{D}{h} \tag{10}$$

When $\tau_s \to 0$, Equation (8) shows that $POW_{cr} \to 0$. In this case, even for a small power loss on the channel i.e. even for a small ΔPOW, the value of the interfacial slipping velocity $\bar{u}$ will be very large and this will generate a large volume flow rate through the channel. This phenomena has actually been observed in the experiments (Majumder et al., 2005; Secchi et al., 2016).

Equation (9) shows that for given τ_s, Δl and r_0 values, the power loss difference ΔPOW is directly proportional to the interfacial slipping velocity $\bar{u}$. It shows that in the case of the interfacial slippage, ΔPOW is only used to generate the interfacial slipping velocity $\bar{u}$, which is very helpful for the mass transfer through the channel. Experiments (Majumder et al., 2005 ; Secchi et al., 2016) also observed the benefits of low friction (i.e. low τ_s) carbon nanotubes, which generated very large flow rates.

Conventional continuum flow theory gives the following critical power loss per unit contact length on the studied channel for initiating the interfacial slippage on the wall surface:

$$POW_{cr,conv} = \frac{\Delta l (h + 2h_{bf,A})^3}{12\eta} \left(\frac{\tau_s}{\frac{1}{2}h + D(n-1)}\right)^2 \tag{11}$$

It is obtained that $r_{cp} = POW_{cr}/POW_{cr,conv} = r_{p,ns}$.

4. CALCULATION

In the calculation, it was taken that $\Delta x/D = 0.15$, $\Delta_{n-2}/D = 0.15$, $\Delta_{j+1}/\Delta_j = q_0 (> 1)$, and $\eta_{line,i}/\eta_{line,i+1} = q_0^m$, where q_0 and m are respectively positive and constant (Zhang, 2019).

It was formulated that (Zhang, 2014):

$$Cy(H_{bf}) = \frac{\eta_{bf}^{eff}(H_{bf})}{\eta} = a_0 + \frac{a_1}{H_{bf}} + \frac{a_2}{H_{bf}^2} \tag{12}$$

where $H_{bf} = h_{bf,A}/h_{cr,bf}$, $h_{cr,bf}$ is a critical thickness, and a_0, a_1 and a_2 are respectively constant and their values are shown in Table 1.

The weak, medium and strong fluid-wall interactions considered respectively have the following characteristic parameter values: Weak interaction: m=0.5, n=3, $q_0 = 1.03$, $h_{cr,bf} = 7nm$.; Medium interaction: m=1.0, n=5, $q_0 = 1.1$, $h_{cr,bf} = 20nm$; Strong interaction: m=1.5, n=8, $q_0 = 1.2$, $h_{cr,bf} = 40nm$.

Table 1 Fluid viscosity data for different fluid-wall interaction types (Zhang, 2014)

Parameter / Interaction	a_0	a_1	a_2
Strong	1.8335	-1.4252	0.5917
Medium	1.0822	-0.1758	0.0936
Weak	0.9507	0.0492	1.6447E-4

5. RESULTS

Figure 2 shows the calculated values of $r_{p,ns}$ and r_{cp} respectively for the weak, medium and strong fluid-wall interactions. These values are all lower than unity. It means that in the case of no wall slippage, for the same operating conditions, the effect of the adsorbed layer reduces the power loss on the studied channel. This is due to the reduction of the volume flow rate through the channel by the adsorbed layer effect. Stronger the fluid-wall interaction, lower values of $r_{p,ns}$ and r_{cp}, and

correspondingly smaller the volume flow rate through the channel and the power loss on the channel. The values of $r_{p,ns}$ and r_{cp} are rapidly reduced with the increase of λ_{bf} i.e. with the reduction of the continuum fluid film thickness h for all the three fluid-wall interactions. This indicates that with the reduction of h, the effect of the adsorbed layer is normally significantly increased. Even for $\lambda_{bf} = 0.02$, we should normally observe the considerable adsorbed layer effect according to Fig.2. This corresponds to the cases of $h_{bf,A} = 2nm, h = 100nm$ or $h_{bf,A} = 1nm$ and $h = 50nm$, where the fluid flow is mainly continuum. It may suggest that we still can not directly draw that the fluid flow enters the non-continuum regime if we detect the deviating results from conventional continuum flow theory in microchannel flows; For such cases, a multiscale approach may be required to simulate the channel flow by incorporating the physical adsorbed layer effect. For $\lambda_{bf} > 0.1$, different fluid-wall interactions have quite different effects on the power loss on the channel according to the significantly different values of $r_{p,ns}$.

In the case of wall slippage, Figure 2 shows that the critical power loss on the channel for initiating the wall slippage is reduced owing to the adsorbed layer effect; Stronger the fluid-wall interaction, lower the value of r_{cp}. However, it may still not be concluded that when the fluid-wall interaction is stronger, the wall slippage in microchannel flows will be more easily generated by a smaller driving power since in this case the value of the interfacial shear strength τ_s will also be increased. Nevertheless, the obtained results strongly suggest that when studying the wall slippage in microchannel flows, the effect of the adsorbed layer on the channel wall surface should be considered by a multiscale approach.

Figure 3 shows the values of r_0, which are actually not influenced by the fluid molecule diameter D, for different fluid-wall interactions. Equation (9) shows that the value of r_0 influences the proportionality of the interfacial slipping velocity $\bar{u}$ to the power loss difference ΔPOW. For given τ_s and Δl, lower the value of r_0, greater the proportionality of $\bar{u}$ to ΔPOW. Figure 3 indeed shows the low values of r_0 which are on the scale of 0.01. Equation (10) shows that the value of r_0 reflects the non-continuum effect of the adsorbed layer. It is also found that for the same continuum fluid film thickness h, the values of r_0 are very close respectively for the weak, medium and strong fluid-wall interactions. For a given fluid-wall interaction, with the reduction of h i.e. with the increase of λ_{bf}, the value of r_0 is monotonously increased.
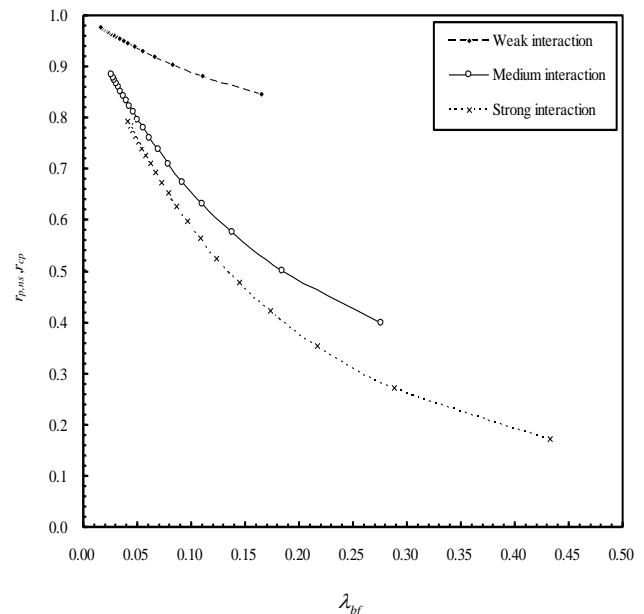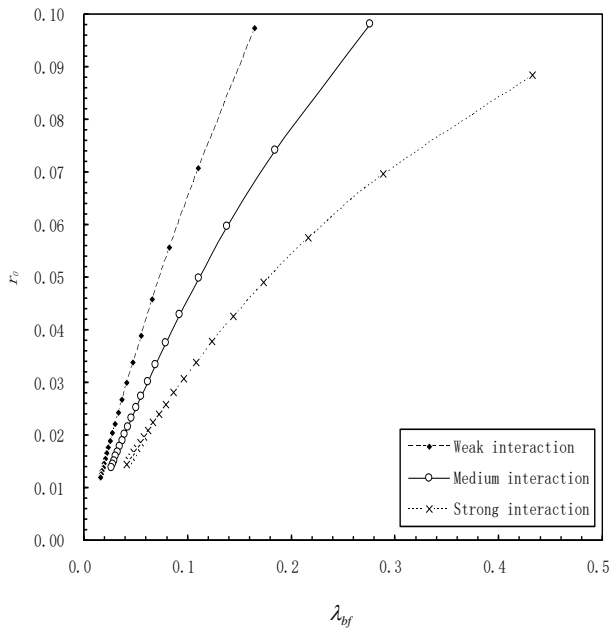

Fig. 2 Values of $r_{p,ns}$ and r_{cp}.

Fig. 3 Values of r_0.

6. CONCLUSIONS

The power loss in a micro slit pore flow is calculated by a multiscale approach to account for both the flow of the physical adsorbed layer on the wall surface and the flow of the intermediate continuum fluid. The flow factor approach model for nanoscale flow was used to model the adsorbed layer flow, and a conventional continuum Newtonian flow theory modeled the continuum fluid flow. The adsorbed layer-wall surface interfacial slippage was assumed, but the adsorbed layer-continuum fluid interfacial slippage was ignored.

The equations for the power loss per unit contact length on the studied channel were derived respectively for no wall slippage and for the wall slippage occurrence. It was found that in the case of no wall slippage, for a given operating condition, the power loss on the channel is significantly reduced by the adsorbed layer effect because of the reduced volume flow rate through the channel; There are the critical power loss on the channel for initiating the wall slippage, which is reduced by the adsorbed layer effect; In the case of the wall slippage, the applied power loss difference from the critical power loss is just used to increase the interfacial slipping velocity, which is very helpful for the mass transfer through the channel; For low friction channel walls, it can be realized only by applying a small power loss on the channel to generate large flow rates through the channel, through generating the high interfacial slipping velocities.

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