Supplementary Material

A review of CFD simulation in pressure driven membrane with fouling model and anti-fouling strategy

Shiyong Miao [a], Jiaying Ma [a], Xuefei Zhou [a, b], Yalei Zhang [a, b], Huaqiang Chu [a, b] *

a State Key Laboratory of Pollution Control and Resource Reuse, Tongji University, Shanghai, 200092, China
b Shanghai Institute of Pollution Control and Ecological Security, Tongji University, Shanghai, 200092, China

* Corresponding author.

E-mail addresses: chuhuaqiang@tongji.edu.cn

1 Dimensionless quantity

1.1 Reynolds number

Reynolds number is the most common dimensionless number used to characterize fluid flow in the feed channel of membrane filtration device. The common formulation of Re is shown as following:

$$Re = \frac{\rho u D}{\mu} \tag{A1}$$

where ρ is the density, μ the dynamic viscosity, D the characteristic length of module and u the fluid velocity in flow channel. The latter two parameters have many variations depending on the actual situation in practice. The most commonly used hydraulic Reynolds number ($\mathrm{Re_h}$) is specified by u_{eff} and D_h.

$$\mathrm{Re_h} = \frac{\rho u_{eff} D_h}{\mu} \tag{A2}$$

where $u_{eff} = u_0/\epsilon$ is the effective flow velocity, u_0 the inlet velocity, ε the porosity and D_h the hydraulic diameter. Compared to u as an engineering control parameter, the effective velocity characterizes the 'sweeping velocity' or 'bulk average velocity' which explain the flow process mechanism of fluid in the channel. It's worth noting that the effective flow velocity (u_{eff}) is grouped with the average velocity in channel (u_{avg}) for convenience due to similar definition in this paper. (Koutsou & Karabelas, 2015) surveyed that the velocity in feed channel shouldn't exceed $0.35\mathrm{m/s}$ due to the manufactory requirements. (Araújo *et al.*, 2012; Bucs *et al.*, 2014) pointed that the actual velocity varies from $0.07\mathrm{m/s}$ to $0.20\mathrm{m/s}$ and frequently value of the inlet velocity is $0.163\mathrm{m/s}$. **Table S1** introduces the characteristic length and velocity used in Reynolds number.

Table S1 The characteristic length and velocity used in Reynolds number

	Effective velocity	Superficial (inlet) velocity
Channel height	(In Seok Kang & Ho Nam Chang, 1982; Li *et al.*, 2002)	(Kerdi *et al.*, 2021; Koutsou *et al.*, 2018; Qamar *et al.*, 2019)*
Filament diameter	(Koutsou *et al.*, 2007; Schwinge *et al.*, 2002)	(Koutsou & Karabelas, 2015)

*for (Koutsou *et al.*, 2018), the characteristic length is modified channel height (channel height-fouling layer thickness), and superficial velocity is got in the channel of gap (channel height-2×fouling layer thickness)

As a widely used engineering parameter, the hydraulic diameter is generally defined as four times the ratio of cross-sectional area to wet circumference.

In the membrane module, the hydraulic diameter in spacer-filled channel should take filaments into account:

$$D_h = \frac{4 \times cross-section\ of\ feed\ channel}{wetted\ circumference} = \frac{4 \times (V - V_f)}{S_m + S_f} \tag{A3}$$

where V is the total channel volume, V_f the filament volume, S_m the membrane surface area, S_f the filament surface area.

Combined with the definition of filaments porosity $\varepsilon = (V - V_f)/V$, the above equation can be converted to:

$$D_h = \frac{4\varepsilon}{2(\mathrm{B+H})/\mathrm{BH} + (1-\varepsilon)\mathrm{SA}} \tag{A4}$$

where $SA = S_f/V_f$, is the specific surface of the spacer, B the channel width, H the channel height (or thickness). The above equation can be simplified for numerical calculation concerning $H \ll B$ in the flow channel. (Kavianipour *et al.*, 2017; Qamar *et al.*, 2019; Schock & Miquel, 1987; Schwinge *et al.*, 2002, 2004)

$$D_h = \frac{4\varepsilon}{2/\mathrm{H} + (1-\varepsilon)\mathrm{SA}} \tag{A5}$$

The Reynolds number has some variations depending on the velocity and characteristic length used listed in **Table S1** The characteristic length and velocity used in Reynolds number: When using the flow channel height as the characteristic length, not only can the calculation be simplified, but the numerical derivation shows that Re is independent of the channel height H and is only determined by the inlet flow rate Q. Therefore, it is possible to compare the effect of different combinations of Re and channel height (the fouling flow channel can simply be considered narrower) on the results.(Koutsou *et al.*, 2018)

Under typical conditions in spirally-wound membrane elements, the velocity in the flow channels between two membrane leaves does not exceed 0.4 (or 0.35) m/s and the manufacturer's recommended operating pressure drop should not exceed 0.6 bar/m. Therefore, the feed flow with Re varying between 50 and 200 is generally considered as laminar flow and tends to transient or unsteady as Re lies between 200 and 600. (Kavianipour *et al.*, 2017; Koutsou *et al.*, 2007, 2018; Koutsou & Karabelas, 2015)

1.2 Sherwood number (Sh)

The Sherwood number is characterized as the ratio of convective to diffusive mass transfer:

$$Sh = \frac{kD}{D_s} \tag{A6}$$

where k is the mass transfer coefficient and D_s the diffusivity. Sherwood number is markedly impacted by Reynolds number and feed channel geometry while (Toh *et al.*, 2020) concluded that the choice of feed concentration has less importance on calculation of Sh for impermeable wall.

1.3 Schmidt number (Sc)

The Schmidt number is used to describe fluids with both momentum and mass diffusion, and is related to the relative thickness of the hydrodynamic and mass transfer boundary layers. In general, higher solute Schmidt number leads to thinner concentration boundary layer.

$$Sc = \frac{\mu}{\rho D_s} \tag{A7}$$

Typical Schmidt number values for the systems of practical interest (i.e., saline waters) in spiral wound elements supposed to be of order 10^3 (1200-5500 measured in experiment depending on fluid properties). However, such a high Sc number result in critically thin concentration boundary layer, which requires finer boundary layer grid to achieve the accuracy requirement. Researchers were forced to lower Sc to 1-100 to perform calculations due to computer limitation (Fimbres-Weihs & Wiley, 2007; Koutsou *et al.*, 2009, 2018; Koutsou & Karabelas, 2015; Li *et al.*, 2002).

1.4 Power number (Pn)

The performance of the spacer can be compared by the mechanical power consumption per m^3 flow channel, namely the specific power consumption (SPC)

$$\text{SPC} = \frac{\Delta P u_{eff} A}{LA} = \frac{\Delta P}{L} u_{eff} \tag{A8}$$

where $\Delta P/L$ is the pressure drop per unit length in the main flow direction and A the cross-section area of flow channel. The pressure drop in feed channel shouldn't exceed $0.6\mathrm{bar/m}$ due to the manufactory requirements (Koutsou & Karabelas, 2015).

Building on this can lead to the Power number (Pn) which represents power consumption in a membrane module.

$$Pn = SPC\frac{\rho^2 H^4}{\mu^3} = EuRe^3\left(\frac{H}{L}\right)\left(\frac{H}{D_h}\right)^3 \tag{A9}$$

Therefore Pn can be interpreted as: $\left(\frac{pressure\ forces}{inertial\ forces}\right) \times \left(\frac{inertial\ forces}{viscous\ forces}\right)^3 \times (geometrical\ ratios)$ (Kavianipour *et al.*, 2017; Li *et al.*, 2002).

1.5 Spacer Configuration Efficacy (SCE)

Since the Sherwood number represents the mass transfer effect and the Power number represents the power consumption, the ratio of the two dimensionless number can be used as an indication for the comparison of the spacer performance with different configurations.

$$SCE = Sh/Pn \tag{A10}$$

Collectively, a relatively high SCE means better mass transfer, lower energy consumption, and thus better performance, possibly associated with reduced concentration polarization effects. (Kavianipour *et al.*, 2017; Koutsou & Karabelas, 2015)

1.6 CP modulus

The CP modulus has been used to measure the degree of CP on the membrane walls. There are several definitions of CP modulus M_{CP} in past studies (Geraldes *et al.*, 2002; Gu *et al.*, 2017a, 2021):

$$M_{CP} = \frac{c_m}{c_f} \text{ or } \frac{c_m - c_0}{c_0} \text{ or } \frac{c_m - c_p}{c_0 - c_p} \quad \text{(A11)}$$

where c_f is the bulk concentration taken from the centroid of the fluid domain in feed channel, c_m the concentration at membrane surface, c_0 the inlet concentration. In general, CP modulus is deformation of the ratio of solute concentration at membrane surface to solute concentration in feed channel.

(Gu *et al.*, 2021) developed a correlation between CP modulus and dimensionless number:

$$M_{CP} = 1 + CRe_c^{\alpha}(m \cdot Re_t)^{\beta} Sc^{\gamma} (\frac{L_f}{D_f})^{\delta} \quad \text{(A12)}$$

where C, α, β, γ, and δ are coefficient and exponents that are dependent on the spacer configuration. Re_c and Re_t is calculated from cross velocity and transmembrane velocity, respectively.

2 Sheer stress

Wall shear stress on the surface of the spacer and membrane is an important characterization indicator of spacer performance and membrane fouling, including biofouling and concentration polarization. High shear stress on the membrane surface mitigates concentration polarization. Nevertheless, bacterial attachment tends to occur in regions of high shear stress as well, followed by microbial proliferation and expansion to region of low shear stress, especially in desalination pre-treatment processes like UF and NF where the feed is biologically active. This compound mechanism suggests that shear stress has an important influence on membrane fouling, thus sheer stress worked as a proxy in membrane evaluation. (Abid *et al.*, 2017; Kerdi *et al.*, 2021; Koutsou *et al.*, 2007; Koutsou & Karabelas, 2015; Lecuyer *et al.*, 2011; Liang *et al.*, 2018; Qamar *et al.*, 2019; Saur *et al.*, 2017)

The magnitude of the wall-tangential shear stress is calculated by taking into account the rate of change of each of the velocity components in the direction away from the wall surface (n): $\tau_i = \mu\,(\partial u_i/\partial n)$ i = x, y, z, while excluding the rate of change of the normal velocity component $(\vec{u} \cdot \vec{n})$ (Liang *et al.*, 2019):

$$\tau_t = \sqrt{\tau_x^2 + \tau_y^2 + \tau_z^2 - \left(\mu \frac{\partial \vec{u}}{\partial n} \cdot \vec{n}\right)^2} \tag{A13}$$

where $\vec{n}$ is a unit vector normal to the wall.

3 Pressure drop & Friction coefficient

The channel pressure drop along the feed channel is an important characteristic which directly related to the pumping energy consumption. With filtration unit operation, significant increase appears in feed channel pressure drop due to module fouling. Meanwhile pressure drop definitely increases as the cost of turbulence promotion. (Ghaffour *et al.*, 2004; Lin *et al.*, 2020; Qamar *et al.*, 2019, 2021).

The correlation between friction factor f and pressure drop $\frac{dp}{dx}$ are shown as following (Gu *et al.*, 2021; Koutsou *et al.*, 2018; Li *et al.*, 2002; Liang *et al.*, 2019; Qamar *et al.*, 2019; Schwinge *et al.*, 2004):

$$f = \frac{\mathrm{D}}{\rho u^2}\frac{dp}{dx} = Eu\frac{D}{L} \tag{A14}$$

Compared to overall pressure drop calculated from the differential inlet and outlet pressure, pressure distribution profile along the flow path outweigh while unachievable due to a lack of the high-precision pressure transducers that detect small differences in pressure. Therefore, CFD simulation works (Xie *et al.*, 2014).

4 Mass transfer coefficient

The mass transfer coefficient k can be explained using film theory (Gu *et al.*, 2017b; McCutcheon & Elimelech, 2006):

$$k = \frac{ShD_s}{d_h} = \frac{1}{C_{\mathrm{f}} - C_{\mathrm{m}}}\left(-D_s\frac{\partial C}{\partial y}\right)_{\mathrm{wall}} \tag{A15}$$

where D_s is the salt diffusion coefficient, d_h the fouling layer thickness, C the solute concentration and subscripts f, m represent the feed channel and membrane surface.

(Koutsou *et al.*, 2018) pointed out that k during the desalination process tends to contribute insignificantly to the overall mass transfer K_t, only 1–2% of the total mass transfer variation is due to an increase of coefficient k, because of channel-gap reduction. Therefore, there is no need to calculate k precisely.

5 Colloidal particle model

The critical flux J_{crit} consider both Brownian diffusion $J_{crit,br}$ and shear-induced diffusion $J_{crit,sh}$ and the particle diffusion coefficient D_p can be similarly divided into two parts (Green & Belfort, 1980; Huisman & Trägårdh, 1999; Topping, 1956; TRETTIN & DOSHI, 1980; Wiesner & Chellam, 1992; ZYDNEY & COLTON, 1986):

$$J_{crit} = \sqrt{J_{crit,br}^2 + J_{crit,sh}^2} \tag{A 16}$$

$$D_p = D_{br} + D_{sh} \tag{A 17}$$

	$\mathrm{J_{crit}}$	D_p
Brownian diffusion	$\mathrm{J_{crit,br}} = 1.31\left(\frac{\dot{\gamma} D_{p-br}^2}{L}\right)^{1/3} \ln\left(\frac{\phi_{c,m}}{\phi_{c,b}}\right)$	$D_{p-br} = \mathrm{kT}/3\pi\mu \mathrm{d_p}$
shear-induced diffusion	$\mathrm{J_{crit,sh}} = 0.078\dot{\gamma}\left(\frac{\mathrm{d_p^4}}{16L}\right)^{1/3} \ln\left(\frac{\phi_{c,m}}{\phi_{c,b}}\right)$	$D_{p-s\hbar} = 0.0075\dot{\gamma}\mathrm{d_p^2}$

where $\dot{\gamma}$ is the shear rate, L is membrane length, $\phi_{c,m}$ is particle volume fraction at the membrane surface, $\phi_{c,b}$ is particle volume fraction at bulk flow, $\mathrm{d_p}$ is particle diameter, k is the Boltzmann constant, T is the fluid temperature and μ is the fluid viscosity.

Particle deposition ratio θ is determined by shear rate as shown in followings (Chong *et al.*, 2008):

$$\theta = \begin{cases} 1 & \dot{\gamma} < 214.29 \\ 1.2502 - 1.1617 \times 10^{-3}\dot{\gamma} & 214.29 < \dot{\gamma} < 214.29 \\ 0.0993 & \dot{\gamma} > 985.71 \end{cases} \tag{A 18}$$

The colloidal particle is the major fouling in MF/UF systems, while rarely be found in NF/RO system as a post-unit. (Vrouwenvelder *et al.*, 2009) confirmed that critical flux concept is not valid for biofouling in NF/RO.

6 References

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